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By: Christine Manchester

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NEW PATENT APPLICATION TRANSMITTAL

- Transmitted herewith for filing is a:
 - (a) [X] utility patent application converted from U.S. Provisional Application Serial Nos. 60/079,965, filed March 30, 1998 and 60/113,146, filed December 16, 1998.
 - [] design patent application
 [] plant patent application
 - (b) Inventor(s): John D. Baxter; Beatrice Darimont; Weijun Feng; Robert J. Fletterick; Peter J. Kushner; Richard L. Wagner; Brian L.

West: and Keith R. Yamamoto

For: METHODS AND COMPOUNDS FOR MODULATING NUCLEAR RECEPTOR COACTIVATOR BINDING

(c) [X] 19 sheets of formal drawing(s).

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METHODS AND COMPOUNDS FOR MODULATING NUCLEAR RECEPTOR COACTIVATOR BINDING

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INTRODUCTION

Technical Field

The present invention relates to methods and compounds for modulating nuclear receptor coactivator binding.

Background

Cells contain receptors that can elicit a biological response by binding various molecules including proteins, hormones and/or drugs. Nuclear receptors represent a super family of proteins that are hormone/ligand-activated transcription factors that enhance or repress transcription in a cell type-, ligand- and promoter-dependent manner. The nuclear receptor family includes receptors for glucocorticoids (GRs), androgens (ARs), mineralocorticoids (MRs), progestins (PRs), estrogens (ERs), thyroid hormones (TRs), vitamin D (VDRs), retinoids (RARs and RXRs), peroxisomes (XPARs and PPARs) and icosanoids (IRs). The so-called "orphan receptors" for which ligands have not been identified are also part of the nuclear receptor superfamily, as they are structurally homologous to the classic nuclear receptors, such as steroid and thyroid receptors.

Although overall sequence conservation between nuclear receptors varies between different families of receptors, sequence conservation between functional regions, or modules, of the receptors is high. For example, nuclear receptors can be organized into functional modules comprising an N-terminal transcriptional activation domain, a central DNA binding domain (DBD), and a C-terminal ligand binding domain (LBD). The LBD of nuclear receptors represents a hormone/ligand-dependent molecular switch. Binding of hormone to a nuclear receptor's LBD changes its ability to modulate transcription of DNA, although they may have transcription-independent actions. Nuclear receptors also bind proteins, such as chaperone complexes, corepressors, or coactivators, that are involved in receptor function. Hormone binding by a nuclear receptor can increase or decrease binding affinity to these proteins, and can influence or mediate the multiple actions of the nuclear receptors on transcription. For example, nuclear receptors can stimulate transcription in response to hormone binding by recruiting coactivator proteins to promoters of responsive genes (Glass et al., Curr. Opin. Cell Biol. (1997) 9:222-32); and Horwitz et al., Mol. Endocrinol. (1996) 10:1167-77).

Coactivators of the p160 family mediate activity of a transcriptional activation domain, called AF2, that is part of the nuclear receptor's LBD. A few receptor mutants deficient in coactivator-dependent activation have been isolated (TR: Collingwood et al. *Proc. Natl. Acad. Sci.* (1997) 94:248-253; VDR: Jurutka et al., J. Biol. Chem. (1997) 227:14592-14599, Masayama et al., Mol. Endocrinol. (1997) 17:1507-1517; ER and RAR: Henttu et al., Mol. Cell Biol. (1997) 17:1832-1839). While these studies support the physiological relevance of the observed interaction, the structural and functional nature of the site to which coactivators bind has not been defined.

The medical importance of nuclear receptors is significant. They have been implicated in breast cancer, prostate cancer, cardiac arrhythmia, infertility, osteoporosis, hyperthyroidism, hypercholesterolemia, obesity and other conditions. However, limited treatments are available and current agonist/antagonist drugs used to target nuclear receptors are ligands that bind to the receptor's LBD buried deep within the receptor. Although additional targets on nuclear receptors are desired for drug development, the structural and functional basis of such sites, including the coactivator binding site, has not been described.

Accordingly, a need exists for identification and characterization of the coactivator binding sites of nuclear receptors, and molecules that affect their interaction with cellular coactivator proteins. This would provide a major new target for iterative drug design, synthesis, and selection. It also would be advantageous to devise methods and compositions for reducing the time required to discover compounds that target the coactivator binding site of nuclear receptors and administer them to organisms to modulate physiological processes regulated by nuclear receptors.

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5 Relevant Literature

Wagner et al., (Nature (1995) 378:690-697) disclose the crystal structure of rat TR-alpha LBD. Various references disclose mutations in carboxyl-terminal helices of nuclear receptors (Henttu et al., supra; O'Donnell et al., Mol. Endocrinol. (1991) 5:94-99; Whitfield et al., Mol. Endocrinol. (1995) 9:1166-79; Saatcioglu et al., Mol. Cell Biol. (1997) 17:4687-95; Collingwood et al., supra; Kamei et al., Cell (1996) 85:403-14). Hong et al. (Proc. Natl. Acad. Sci. USA (1996) 93(10):498-49452) and Hong et al. (Mol. Cell. Biol. (1997) 17:2735-2744) disclose cloning and expression of GRIP1 coactivator. Torchia et al., (Nature (1997) 387:677-84), Le Douarin et al., (EMBO J (1996) 15:6701-6715) and Heery et al. (Nature (1997) 387:733-736) disclose sequence alignment of various coactivator proteins showing a (SEQ ID NO: 1) LxxLL motif.

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SUMMARY OF THE INVENTION

The present invention relates to identification and manipulation of the coactivator binding site of nuclear receptors. Identification of this site permits design and obtention of compounds that bind to the coactivator binding site of nuclear receptors and modulate coactivator binding to the receptor. The compounds include agonists and antagonists that modulate nuclear receptor activity by promoting (agonists) or blocking (antagonists) hormone-dependent coactivator binding to the receptor, particularly antagonists. The compounds of the invention can be receptor-, cell- and/or tissue-specific.

The present invention also includes protein cocrystals of nuclear receptors with a molecule bound to the coactivator binding site and methods for making them. The cocrystals provide means to obtain atomic modeling information of the specific amino acids and their atoms forming the coactivator binding site and that interact with molecules that bind to the site, such as coactivator. The cocrystals also provide modeling information regarding the coactivator:nuclear receptor interaction, as well as the structure of coactivators bound thereto.

The present invention further provides methods for identifying and designing small molecules that bind to the coactivator binding site using atomic models of nuclear receptors. The method involves modeling test compounds that fit spacially into a nuclear receptor coactivator binding site of interest using an atomic structural model comprising a nuclear receptor coactivator binding site or portion thereof, screening the test compounds in a biological assay characterized by binding of a test compound to a nuclear receptor coactivator binding site, and identifying a test compound that modulates coactivator binding to the nuclear receptor.

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The invention also includes compositions and methods for identifying coactivator binding sites of nuclear receptors. The methods involve examining the surface of a nuclear receptor of interest to identify residues that modulate coactivator binding. The residues can be identified by homology to the coactivator binding site of human TR described herein. Overlays and superpositioning with a three dimensional model of a nuclear receptor LBD, or a portion thereof that contains a coactivator binding site, also can be used for this purpose. Additionally, alignment and/or modeling can be used as a guide for the placement of mutations on the LBD surface to characterize the nature of the site in the context of a cell.

Also provided is a method of modulating the activity of a nuclear receptor. The method can be *in vitro* or *in vivo*. The method comprises administering, *in vitro* or *in vivo*, a sufficient amount of a compound that binds to the coactivator binding site. Preferred compounds bind to the site with greater affinity than coactivator proteins found in a cell of interest. Binding at this site, the compound can compete for binding of coactivator proteins, thereby inhibiting gene transcription, or in some cases promoting it, even when hormone is or is not bound.

The invention further includes a method for identifying an agonist or antagonist of coactivator binding to a nuclear receptor. The method comprises providing the atomic coordinates comprising a nuclear receptor coactivator binding site or portion thereof to a computerized modeling system; modeling compounds which fit spacially into the nuclear receptor coactivator binding site; and identifying in an assay for nuclear receptor activity a compound that increases or decreases activity of the nuclear receptor through binding the coactivator binding site.

Also provided is a machine-readable data storage medium with information for constructing and manipulating an atomic model comprising a coactivator binding site or portion thereof. The medium comprises a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of a molecule or molecular complex for a nuclear receptor coactivator binding site.

Also provided is a method of identifying a compound that selectively modulates the activity of one type of nuclear receptor compared to other nuclear receptors. The method is exemplified by modeling test compounds that fit spacially and preferentially into a nuclear receptor coactivator binding site of interest using an atomic structural model of a nuclear receptor coactivator binding site, selecting a compound that interacts with one or more residues of the coactivator binding site unique in the context of that site, and identifying in an assay for coactivator binding activity a compound that selectively binds to the coactivator binding site compared to other nuclear receptors.

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5 The unique features involved in receptor-selective coactivator binding can be identified by comparing atomic models of different receptors or isoforms of the same type of receptor.

The invention finds use in the selection and characterization of peptide, peptidomimetic, as well as other small molecule compounds, such as small organic molecules, identified by the methods of the invention, particularly new lead compounds useful in treating nuclear receptor-based disorders.

BRIEF DESCRIPTION OF THE DRAWINGS

Figure 1 shows the specific effects of mutations on hTRβ1 transcriptional activation in HeLa cells and correlation with effects on binding to GST-GRIP1. T₃ dependent activation of transcription of a reporter gene, expressed as the percentage of WT is plotted for each mutant. GST-GRIP1 binding, analyzed by autoradiography after separation using 10% SDS-PAGE, was also expressed as the percentage of WT and plotted for each mutant. The GST-GRIP1 used included GRIP1 amino acids 721-1121; the same results were obtained using a GST-GRIP1 construct including GRIP1 amino acids 563-1121 (data not shown).

Figure 2 shows that overexpression of full-length GRIP1 rescues loss of transcriptional activation by hTRβ1 mutants. Indicated amounts of the expression vector for full-length GRIP1, pSG5-GRIP1, is included in the cotransfections, which otherwise are performed as in Figure 1. The WT or different representative hTRβ1 mutants are indicated.

Figure 3 shows specific hERα surface mutants cause loss of transcriptional activation in
42. HeLa cells in parallel with their loss of in vitro GRIP1 binding. The fold E₂ activation, expressed as the percentage of WT, and the phosphorimager quantitation of in vitro binding of [35S]-labeled hERα WT and mutants to GST-GRIP1 (GRIP1 amino acids 721-1121) also expressed as the percentage of WT is plotted for each mutant.

Figure 4 shows a plot of the fold E₂ activation observed when the indicated amounts of the full-length GRIP1 expression vector, pSG5-GRIP1, are added to the co-transfection experiment, which otherwise is performed as for Figure 3. The WT or different hERα mutants are indicated.

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5 The data represent the averages of three independent experiments, with standard deviations less than 10%

Figure 5 shows a CPK model of the $TR\alpha$ -LBD, indicating the LBD surface locations of mutations made in the full-length hTR β 1. Mutated residues having no effect on GRIP1 binding or effect on activation in HeLa cells are shaded gray. Mutated residues with diminished GRIP1 and SRC-1a binding and diminished activation in HeLa cells are colored to reflect chemical properties of the residues: red, blue (purple), and green indicate acidic, basic, and hydrophobic residues, respectively. The main chain structures of the $TR\alpha$ - and $TR\beta$ -LBDs are the same (data not shown).

Figure 6 shows sequence alignment of amino acid residues of members of the p160 coactivator family. Single amino acid designations are used. Members of the p160 coactivator family interact with the nuclear receptors through conserved (SEQ ID NO: 1) LxxLL motifs.

Figure 7 shows binding affinity assays of GST-GRIP1 constructs with NR-boxes 1, 2, and/or 3 and their interaction with TR LBD. GRIP-1 NR boxes 1,2 and 3 interact differently with TRβ LBD. Single letter designations are used for the amino acids.

Figure 8 shows binding affinity assays of GST-GRIP1 constructs with NR-boxes 1, 2, and/or 3 and their interaction with TR and GR LBDs. TR and GR differ in their interactions with GRIP-1.

Figure 9 shows binding affinity assays for NR-box 2- and 3-peptides and GRIP1 and their interaction with TR LBD. NR box 2- and 3-containing peptides reproduce the affinity and specificity of the NR interaction domain.

Figure 10 shows binding affinity assays for NR-box 2- and 3-peptides and their interaction with TR LBD. Sequence adjacent to the (SEQ ID NO: 1) LxxLL motif modulate the affinity of NR-box-TR β LBD interactions.

Figure 11 shows binding affinity assays for mutant GRIP1 and NR-box 2- and 3-peptides and their interaction with TR LBD. The individual leucine residues of the (SEQ ID NO: 1) LxxLL motif are crucial for binding of the GRIP-1 NR interaction domain to TRB LBD.

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Figure 12 shows the contents of the asymmetric unit of the crystallized hTRB LBD:GRIP1 NR-box 2 peptide complex. The crystal lattice consists of a repeating unit containing a 2:2 complex of hTR LBD and GRIP1 site 2 peptide. Positions of the two GRIP1 site 2 peptides are boxed, in green (site1), and red (site 2), with the peptides drawn as a C-alpha trace. The two NCS related monomers of the hTR LBD are shown as a secondary structure ribbon drawing, with monomer 1 in light grey, and monomer 2 in dark grey. The side chains of the hydrophobic residues I689, L690, L693, L694 of the GRIP1 NR-box 2 peptides are drawn to emphasize those interactions observed in both bound peptides.

Figure 13 shows a ribbon diagram depicting the interaction of the GRIP1 NR-box 2 peptide with the hTR β LBD. The GRIP1 NR-box 2 peptide (dark grey) forms three turns of α -helix, and binds the hTR LBD (light gray) in a hydrophobic cleft defined by helices H3, H4, H5, and H12. Portions of the hTR β LBD, and the neighboring monomer, are omitted for clarity.

Figure 14 shows interface between the GRIP1 NR-box 2 peptide and the hTRß LBD. Side chains of residues of the hTRß LBD within 4.5Å of the GRIP-1 NR-box 2 peptide are labeled. The color of the individual side chains reflects the chemical nature of the residue: acidic residues are red, basic residue are blue, aliphatic residues are green, aromatic residues are brown, and polar residues are orange. The peptide is depicted as a C-alpha trace with the side chains of (SEQ ID NO: 2) ILxxLL motif shown explicitly.

Figure 15 shows residues in the hTRß LBD that are necessary for transactivation. The transactivation mutations are mapped onto the interface between the GRIP1 NR-box 2 peptide and the hTRß LBD

Figure 16 shows molecular surface of the hTR LBD. The side chains of the leucines resides fit within a hydrophobic groove formed from helices H3, H5, and H12, while the side chain of the non-conserved isoleucine residue packs against the outside edge of the groove. The remainder of the peptide is shown as main chain.

Figure 17 shows complementarity between the (SEQ ID NO: 1) LxxLL motif and the surface of the hTR LBD. The side chains of the (SEQ ID NO: 2) ILxxLL motif are shown in a CPK representation, with the main chain of the peptide drawn as a C-alpha trace. The three leucince

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5 residues fit into pockets of the coactivator binding site of the hTRB LBD, depicted as mesh, while the isoleucine residue rests on the edge of the site's cleft.

Figure 18 shows the coactivator binding site cleft, one side of which is formed by conformationally hormone-responsive residues. On the left is a view of the TR-LBD molecular surface showing the concave surfaces in gray. The cavity is shown at the center of the figure. On the right is shown a CPK model of the TR-LBD, overlaid with a molecular surface view, which is restricted to a 12Å radius of the hydrophobic cavity. Mutated residues of the coactivator binding site that are hormone-insensitive (V284, K288, I302 and K306) are located on one side of the cleft and are colored yellow. Mutated CBS residues likely undergo a conformational change upon hormone binding (L454 and E457) are located on the opposite side of the cleft and are colored red.

Figure 19 shows alignment of amino acid sequences (single letter amino acid designations) containing residues that form the coactivator binding sites of several nuclear receptors. The boxes represent residues of alpha-helix (H3, H4, H5, H6 and H12); lower case letters "h" and "q" represent hydrophobic and polar residues, respectively.

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DESCRIPTION OF SPECIFIC EMBODIMENTS

The present invention provides methods and compositions for identifying compounds that modulate nuclear receptor activity. The compounds can be nuclear receptor agonists or antagonists that bind to the coactivator binding site (and that act as mimetics to the coactivator in this regard), and promote (agonists) or block (antagonists) binding of the coactivator to the target nuclear receptor. Compounds that bind to the coactivator binding site also are provided. The compounds can be natural or synthetic. Preferred compounds are small organic molecules, peptides and peptidomimetics (e.g., cyclic peptides, peptide analogs, or constrained peptides).

As described in the Examples, mutagenesis and coactivator binding studies, coupled with analysis of atomic models derived from cocrystals, reveals for the first time a previously unknown structure for nuclear receptors, the coactivator binding site. By "coactivator binding site" is intended a structural segment or segments of nuclear receptor polypeptide chain folded in such a way so as to give the proper geometry and amino acid residue conformation for binding a coactivator. This is the physical arrangement of protein atoms in three-dimensional space forming a coactivator binding site pocket or cavity. Residues forming the site are amino acids corresponding to (i.e., the same as or equivalent to) human TR residues of C-terminal helix 3 (Ile280, Thr281, Val283, Val284, Ala287, and Lys288), helix 4 (Phe293), helix 5 (Gln301, Ile302, Leu305, Lys306), helix 6 (Cvs309), and helix 12 (Leu454, Glu457, Val458 and Phe459). The coactivator binding site is highly conserved among the nuclear receptor super family (Figure 19). Thus, this site corresponds to a surprisingly small cluster of residues on the surface of the LBD that form a prominent hydrophobic cleft. The hydrophobic cleft is formed by hydrophobic residues corresponding to human TR residues of C-terminal helix 3 (Ile280, Val283, Val284, and Ala287), helix 4 (Phe293), helix 5 (Ile302 and Leu305), helix 6 (Cvs309), and helix 12 (Leu454, Val458 and Phe459). The hydrophobic cleft of the coactivator binding site also is highly conserved among the nuclear receptor super family (Figure 19).

The invention also includes compositions and methods for identifying coactivator binding sites of nuclear receptors. The methods involve examining the surface of a nuclear receptor of interest to identify residues that modulate coactivator binding. The residues can be identified by homology to the coactivator binding site of human TR described herein. A preferred method is alignment with the residues of any nuclear receptor corresponding to (i.e., equivalent to) human TR residues of the C-terminal helix 3 (Ile280, Thr281, Val283, Val284, Ala287, and Lys288), helix 4

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5 (Phe293), helix 5 (Gln301, Ile302, Leu305, Lys306), helix 6 (Cys309), and helix 12 (Pro453, Leu454, Glu457, Val458 and Phe459). Overlays and superpositioning with a three-dimensional model of a nuclear receptor LBD, or a portion thereof that contains a coactivator binding site, also can be used for this purpose. For example, three-dimensional structures of TR, RAR, RXR and ER LBDs can be used for this purpose. For example, nuclear receptors identifiable by homology alignment include normal nuclear receptors or proteins structurally related to nuclear receptors found in humans, natural mutants of nuclear receptors found in humans, normal or mutant receptors found in animals, as well as non-mammalian organisms such as pests or infectious organisms, or viruses.

Alignment and/or modeling also can be used as a guide for the placement of mutations on the LBD surface to characterize the nature of the site in the context of a cell. Selected residues are mutated to preserve global receptor structure and solubility. To destroy the coactivator binding interaction, preferred mutations are to charged residues (e.g., Arg, Lys, or Glu) on the basis that bulky, surface charged residues might disrupt coactivator binding, yet preserve global receptor structure and solubility. Mutants can be tested for coactivator binding as well as the relative change in strength of the binding interaction. Ligand-dependent coactivator interaction assays also can be tested for this purpose, such as those described herein.

Compounds that bind to the coactivator binding site of nuclear receptors can be identified by computational modeling and/or screening. For example, coactivator agonists or antagonists can be identified by providing atomic coordinates comprising a nuclear receptor coactivator binding site or portion thereof to a computerized modeling system, modeling them, and identifying compounds that fit spacially into the coactivator binding site. By a "portion thereof" is intended the atomic coordinates corresponding to a sufficient number of residues or their atoms of the coactivator binding site that interact with a compound capable of binding to the site. This includes receptor residues having an atom within 4.5Å of a bound compound or fragment thereof. For instance, human TR residues V284, Phe293, Ile302, Leu305 and Leu454 contain side chain atoms that are within 4.5Å, and interact with, hydrophobic residues of a (SEQ ID NO: 1) LxxLL motif of an NRbox 2 coactivator peptide. As another example, an atomic structural model utilized for computational modeling and/or screening of compounds that bind to the coactivator binding site may include a portion of atomic coordinates of amino acid residues corresponding to the site composed of residues of human thyroid receptor selected from Val284, Lys288, Ile302, Lys306, Leu454 and Glu457, or their structural and functional equivalents found in other receptors. Thus, for example, the atomic coordinates provided to the modeling system can contain atoms of the nuclear receptor LBD, part of the LBD such as atoms corresponding to the coactivator binding site

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5 or a subset of atoms useful in the modeling and design of compounds that bind to a coactivator binding site.

The atomic coordinates of a compound that fits into the coactivator binding site also can be used for modeling to identify compounds or fragments that bind the site. By "modeling" is intended quantitative and qualitative analysis of molecular structure/function based on atomic structural information and receptor-coactivator agonists/antagonists interaction models. This includes conventional numeric-based molecular dynamic and energy minimization models, interactive computer graphic models, modeling is preferably performed using a computer and other structure-based constraint models. Modeling is preferably performed using a computer and may be further optimized using known methods. By "fits spacially" is intended that the three-dimensional structure of a compound is accommodated geometrically by a cavity or pocket of a nuclear receptor coactivator binding site.

Compounds of particular interest fit spacially and preferentially into the coactivator binding By "fits spacially and preferentially" is intended that a compound possesses a threedimensional structure and conformation for selectively interacting with a nuclear receptor coactivator binding site. Compounds that fit spacially and preferentially into the coactivator binding site interact with amino acid residues forming the hydrophobic cleft of this site. In particular, the hydrophobic cleft of the coactivator binding site comprises a small cluster of hydrophobic residues. The site also contains polar or charged residues at its periphery. The present invention also includes a method for identifying a compound capable of selectively modulating coactivator binding to different nuclear receptors. The method comprises the steps of modeling test compounds that fit spacially and preferentially into the coactivator binding site of a nuclear receptor of interest using an atomic structural model of a nuclear receptor, screening the test compounds in a biological assay for nuclear receptor activity characterized by preferential binding of a test compound to the coactivator binding site of a nuclear receptor, and identifying a test compound that selectively modulates the activity of a nuclear receptor. Such receptor-specific compounds are selected that exploit differences between the coactivator binding sites of one type of receptor versus a second type of receptor, such as the differences depicted in Figure 19.

The invention also is applicable to generating new compounds that distinguish nuclear receptor isoforms. This can facilitate generation of either tissue-specific or function-specific compounds. For instance, GR subfamily members have usually one receptor encoded by a single gene, although there are exceptions. For example, there are two PR isoforms, A and B, translated from the same mRNA by alternate initiation from different AUG codons. There are two GR forms,

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one of which does not bind ligand. This method is especially applicable to the TR subfamily which usually has several receptors that are encoded by at least two (TR: α , β) or three (RAR, RXR, and PPAR: α , β , γ) genes or have alternate RNA splicing.

The receptor-specific compounds of the invention preferably interact with conformationally constrained residues of the coactivator binding site that are conserved among one type of receptor compared to a second type of receptor. "Conformationally constrained" is intended to refer to the three-dimensional structure of a chemical or moiety thereof having certain rotations about its bonds fixed by various local geometric and physical-chemical constraints. Conformationally constrained structural features of a coactivator binding site include residues that have their natural flexible conformations fixed by various geometric and physical-chemical constraints, such as local backbone, local side chain, and topological constraints. These types of constraints are exploited to restrict positioning of atoms involved in receptor-coactivator recognition and binding.

For instance, comparison of sequences of the GR and TR coactivator interaction surface shows a highly negatively charged sequence at the C-terminal end of TR helix 12 (E460 and D461) that is neutral in the equivalent positions in GR helix 12 (GR residues T788 and N759, corresponding to TR residue positions 460 and 461, as depicted in Figure 19). As described in the Examples, the cocrystal of the hTRß LBD complexed with the GRIP1 NR-box 2 peptide shows that TR residues E460 and D461 interact with positively charged residues of the NR-box 2 peptide. Also, when comparing the RAR LBD structure to that of the TR LBD, conformation of helix 12 differs slightly, whereas helices 3, 4, 5 and 6 are substantially the same. Thus, differences in helix 12, particularly charge differences at the C-terminal end of the helix, may modulate preferential interaction of TR for NR-box 2 containing coactivators. As further demonstrated in the Examples, TR and GR differ in their specificity for different NR-boxes containing the conserved (SEQ ID NO: 1) LxxLL motif found in members of the p160 family of coactivator proteins. As also demonstrated in the Examples, GR but not TR is able to interact with peptides containing the hydrophobic interaction motifs of p53 (SEQ ID NO: 3; FxxLW) and VP16 (SEQ ID NO: 4; FxxAL). Thus, TR exhibits preferential interaction with NR-box peptides comprising the (SEQ ID NO: 1) LxxLL motif, but GR does not discriminate and can bind peptides containing a generic amphipathic helix motif. Accordingly, these real differences among the various nuclear receptors can be exploited in the identification and design of compounds that modulate coactivator binding to one nuclear receptor compared to another.

For modeling, docking algorithms and computer programs that employ them can be used to identify compounds that fit into the coactivator binding site. For example, docking programs can be

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used to predict how a small molecule of interest can interact with the nuclear receptor coactivator 5 binding site. Fragment-based docking also can be used in building molecules de novo inside the coactivator binding site, by placing chemical fragments that complement the site to optimize intermolecular interactions. The techniques can be used to optimize the geometry of the binding interactions. This design approach has been made possible by identification of the coactivator binding site structure thus, the principles of molecular recognition can now be used to design a 10 compound which is complementary to the structure of this site. Compounds fitting the coactivator binding site serve as a starting point for an iterative design, synthesis and test cycle in which new compounds are selected and optimized for desired properties including affinity, efficacy, and selectivity. For example, the compounds can be subjected to addition modification, such as 15 replacement and/or addition of R-group substituents of a core structure identified for a particular class of binding compounds, modeling and/or activity screening if desired, and then subjected to additional rounds of testing.

Computationally small molecule databases can be screened for chemical entities or compounds that can bind in whole, or in part, to a nuclear receptor coactivator binding site of interest. In this screening, the quality of fit of such entities or compounds to the binding site may be judged either by shape complementarity (DesJalais et al., *J. Med. Chem.* (1988) 31:722-729) or by estimated interaction energy (Meng et al., *J. Comp. Chem.* (1992) 13:505-524). The molecule databases include any virtual or physical database, such as electronic and physical compound library databases, and are preferably used in developing compounds that modulate coactivator binding.

Compounds can be designed intelligently by exploiting available structural and functional information by gaining an understanding of the quantitative structure-activity relationship (QSAR), using that understanding to design new compound libraries, particularly focused libraries having chemical diversity of one or more particular groups of a core structure, and incorporating any structural data into that iterative design process. For example, one skilled in the art may use one of several methods to screen chemical entities or fragments for their ability to associate with the coactivator binding site of a nuclear receptor of interest. This process may begin by visual inspection of, for example, the coactivator binding site on the computer screen. Selected fragments or chemical entities may then be positioned into all or part of the site. Docking may be accomplished using software such as Quanta and Sybyl, followed by energy minimization and molecular dynamics with standard molecular mechanics force-fields, such as CHARMM and AMBER.

For example, compounds and/or fragments can be designed to fill up the hydrophobic cleft, the pocket deep within the cleft, the upper end of the site, and/or the lower end of the site. Residues comprising a coactivator binding site, when defined by the user as those residues having an atom within 4.5Å of an atom of a bound chemical entity, can be modeled to look for energetic contributions and interaction with the bound chemical entity. For example, a compound or fragment can be designed to contain hydrophobic groups that interact with hydrophobic residues of the coactivator binding site. As described in the examples, human TR residues V284, Phe293, Ile302, Leu305 and Leu454 contain side chain atoms that are within 4.5Å, and interact with, hydrophobic residues of a (SEQ ID NO: 1) LxxLL motif of an NR-box 2 coactivator peptide. Thus, for example, peptides and/or peptide mimetics having a hxxhh motif, where "h" is a hydrophobic residue and x is any residue, can be constructed. Small organic molecules that mimic one or more of these particular interactions also can be designed, for example, by including one or more R-groups that are hydrophobic and fit into the site.

Specialized computer programs may also assist in the process of selecting chemical entity fragments or whole compounds. These include: GRID (Goodford, J. Med. Chem. (1985) 28:849-857; available from Oxford University, Oxford, UK); MCSS (Miranker et al., Proteins: Structure, Function and Genetics, (1991) 11:29-34; available from Molecular Simulations, Burlington, MA); AUTODOCK (Goodsell et al., Proteins: Structure, Function and Genetics (1990) 8:195-202; available from Scripps Research Institute, La Jolla, CA); and DOCK (Kuntz et al, J. Mol. Biol. (1982) 161:269-288; available from University of California, San Francisco, CA).

Additional commercially available computer databases for small molecular compounds include Cambridge Structural Database and Fine Chemical Database (Rusinko, *Chem. Des. Auto. News* (1993) 8:44-47).

Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound. Assembly may be proceeded by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of a nuclear receptor. This can be followed by manual model building using software such as Quanta or Sybyl.

Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include: CAVEAT (Bartlett et al., "CAVEAT: A Program to Facilitate the Structure-Derived Design of Biologically Active Molecules", In: *Molecular Recognition in Chemical and Biological Problems*", Special Pub., *Royal Chem. Soc.* (1989) 78:182-196; CAVEAT is available from the University of California, Berkeley, CA); 3D Database systems such as MACCS-3D (MDL

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5 Information Systems, San Leandro, CA; reviewed in Martin, J. Med. Chem. (1992) 35:2145-2154); and HOOK (available from Molecular Simulations. Burlington, MA).

In addition to building a compound in a step-wise fashion, one fragment or chemical entity at a time as described above, compounds that bind to a coactivator binding site of interest also may be designed as a whole or *de novo* using either an empty coactivator binding site or optionally including some portion(s) of a molecule known to binds to the site, such as an NR-box type peptide. These methods include: LUDI (Bohm, *J. Comp. Aid. Molec. Design* (1992) 6:61-78; LUDI is available from Biosym Technologies, San Diego, CA); LEGEND (Nishibata et al., *Tetrahedron* (1991) 47:8985; LEGEND is available from Molecular Simulations, Burlington, MA); and LeapFrog (available from Tripos Associates, St. Louis, MO).

Other molecular modeling techniques may also be employed in accordance with this invention. See, for example, Cohen et al., *J. Med. Chem.* (1990) 33:883-894); Navia et al., *Curr. Opin. Struct. Biol.* (1992) 2:202-210). For example, where the structures of test compounds are known, a model of the test compound may be superimposed over the model of the structure of the invention. Numerous methods and techniques are known in the art for performing this step, any of which may be used. See, for example, Farmer, "*Drug Design*," Ariens, E.J., ed., 10:119-143 (Academic Press, New York, 1980); U.S. Patent No. 5,331,573; U.S. Patent No. 5,500,807; Verlinde, *Structure*, (1994) 2:577-587); and Kuntz et al., *Science*, (1992) 257:1078-1082). The model building techniques and computer evaluation systems described herein are not a limitation on the present invention.

Using these computer modeling systems a large number of compounds may be quickly and easily examined and expensive and lengthy biochemical testing avoided. Moreover, the need for actual synthesis of many compounds can be substantially reduced and/or effectively eliminated.

Compounds identified through modeling can be screened in an assay characterized by binding of the compound to a coactivator binding site of interest for coactivator binding activity, such as a biologically based assay. Screening can be in vitro and/or in vivo. Preferred assays include cell-free competition assays and cell culture based assays. The biological screening preferably centers on activity-based response models, binding assays (which measure how well a compound binds to the receptor), and bacterial, yeast and animal cell lines (which measure the biological effect of a compound in a cell). The assays can be automated for high capacity - high throughput screening (HTS) in which large numbers of compounds can be tested to identify compounds with the desired activity.

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As an example, in vitro binding assays can be performed in which compounds are tested for their ability to block the binding of a coactivator protein, fragment, fusion or peptide thereof, to a coactivator binding site of interest. For cell and tissue culture assays, they may be performed to assess a compound's ability to block function of cellular coactivators, such as members of the p160 family of coactivator proteins, such as SRC-1, AIB1, RAC3, p/CIP, and GRIP1 and its homologues TIF 2 and NcoA-2, and those that exhibit receptor and/or isoform-specific binding affinity. In a preferred embodiment, compounds of the invention bind to a nuclear receptor coactivator binding site with greater affinity than the cellular coactivator proteins. Tissue profiling and appropriate animal models also can be used to select compounds. Different cell types and tissues also can be used for these biological screening assays. Suitable assays for such screening are described herein and in Shibata et al. (Recent Prog. Horm. Res. 52:141-164 (1997)); Tagami et al. (Mol. Cell Biol. (1997) 17(5):2642-2648); Zhu et al. (J. Biol. Chem. (1997) 272(14):9048-9054); Lin et al. (Mol. Cell Biol. (1997) 17(10):6131-6138); Kakizawa et al. (J. Biol. Chem. (1997) 272(38):23799-23804); and Chang et al. (Proc. Natl. Acad. Sci. USA (1997) 94(17):9040-9045), which references are incorporated herein in their entirety by reference. For example, coactivators or binding fragments thereof can be expressed and/or assayed for binding as for GRIP1 (Hong et al., MCB supra; and Hong et al., PNAS supra) and/or SRC-1 (Spencer et al., Nature (1997) 389:194-198; Onate et al., Science (1995) 270:1354-1357), incorporated by reference.

The compounds selected can have agonist and/or antagonistic properties. The compounds also include those that exhibit new properties with varying mixtures of agonist and antagonist activities, depending on the effects of altering coactivator binding in the context of different activities of nuclear receptors, either hormone-dependent or hormone-independent, which are mediated by proteins other than coactivators, and which interact with the receptors at locations other than the coactivator binding site. The compounds also include those, which through their binding to receptor locations that are conformationally sensitive to hormone binding, have allosteric effects on the receptor by stabilizing or destabilizing the hormone-bound conformation of the receptor, or by directly inducing the same, similar, or different conformational changes induced in the receptor by the binding of hormone.

Of particular interest is use of such compounds in a method of modulating nuclear receptor activity in a mammal by administering to a mammal in need thereof a sufficient amount of a compound that fits spatially and preferentially into a coactivator binding site of a nuclear receptor of interest. By "modulating" is intended increasing or decreasing activity of a nuclear receptor. For example, pre-clinical candidate compounds can be tested in appropriate animal models in order to measure efficacy, absorption, pharmacokinetics and toxicity following standard techniques known

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5 in the art. Compounds exhibiting desired properties are then tested in clinical trials for use in treatment of various nuclear receptor-based disorders. These include ER-based disorders, such as postmenopausal symptoms and cancer resulting from loss of estrogen production, and osteoporosis and cardiovascular disease stemming from traditional estrogen replacement therapy. Others include TR-based disorders including cardiovascular disease, metabolic disorders, hyperthyroidism, 10 glaucoma and skin disorders. GR-based disorders include Type II diabetes and inflammatory conditions such as rheumatic diseases.

The invention also provides for cocrystals made from nuclear receptor ligand binding domains with a molecule bound to the coactivator binding site. As exemplified in the Examples, TR LBDs are co-crystallized with a peptide molecule comprising a coactivator NR-box 2 peptide sequence bound to the coactivator binding site, and the hormone/ligand T₃.

Crystals are made from purified nuclear receptor LBDs that are usually expressed by a cell culture, such as *E. coli*. Preferably, different crystals (cocrystals) for the same nuclear receptor are separately made using different coactivators-type molecules, such as protein fragments, fusions or small peptides. The coactivator-type molecules preferably contain NR-box sequences necessary for binding to the coactivator binding site, or derivatives of NR-box sequences. Other molecules can be used in co-crystallization, such as small organics that bind to the coactivator or hormone binding site(s). Heavy atom substitutions can be included in the LBD and/or a co-crystallizing molecule.

After the three dimensional structure of the cocrystal is determined, the structural information can be used in computational methods to design synthetic compounds for the nuclear receptor, and further structure-activity relationships can be determined through routine testing using the assays described herein and known in the art.

Since nuclear receptor LBDs may crystallize in more than one crystal form, the structure coordinates of such receptors or portions thereof, as provided in **Appendix 1**, are particularly useful for solving the structure of those other crystal forms of nuclear receptors. They may also be used to solve the structure of mutants or co-complexes of nuclear receptors having sufficient structural similarity.

One method that may be employed for this purpose is molecular replacement. In this method, the unknown crystal structure, may be determined using the structure coordinates of this invention as provided in **Appendix 1**. This method will provide an accurate structural form for the unknown crystal more quickly and efficiently than attempting to determine such information ab initio

Atomic coordinate information gleaned from the crystals of the invention can be stored. In a preferred embodiment, the information is provided in the form of a machine-readable data storage medium. This medium contains information for constructing and/or manipulating an atomic model of a coactivator binding site or portion thereof. For example, the machine readable data for the coactivator binding site comprises structure coordinates of amino acids corresponding to human TR amino acids selected from C-terminal helix 3 (Ile280, Thr281, Val283, Val284, Ala287, and Lys288), helix 4 (Phe293), helix 5 (Gln301, Ile302, Leu305, Lys306), helix 6 (Cys309), and helix 12 (Pro453, Leu454, Glu457, Val458 and Phe459), or a homologue of the molecule or molecular complex comprising the site. The homologues comprise a coactivator binding site that has a root mean square deviation from the backbone atoms of the amino acids of not more than 1.5Å. A preferred molecule or complex represents a compound bound to the coactivator binding site.

The machine-readable data storage medium can be used for interative drug design and molecular replacement studies. For example, a data storage material is encoded with a first set of machine-readable data that can be combined with a second set of machine-readable data. For molecular replacement, the first set of data can comprise a Fourier transform of at least a portion of the structural coordinates of the nuclear receptor or portion thereof of interest, and the second data set comprises an X-ray diffraction pattern of the molecule or molecular complex of interest. Using a machine programmed with instructions for using the first and second data sets a portion or all of the structure coordinates corresponding to the second data can be determined.

Protein for crystals and assays described herein can be produced using expression and purification techniques described herein and known in the art. For example, high level expression of nuclear receptor LBDs can be obtained in suitable expression hosts such as *E. coli*. Expression of LBDs in *E. coli*, for example, includes the TR LBD and other nuclear receptors, including members of the steroid/thyroid receptor superfamily, such as the receptors ER, AR, MR, PR, RAR, RXR and VDR. Yeast and other eukaryotic expression systems can be used with nuclear receptors that bind heat shock proteins as these nuclear receptors are generally more difficult to express in bacteria, with the exception of ER, which can be expressed in bacteria. Representative nuclear receptors or their ligand binding domains have been cloned and sequenced: human RAR-α, human RAR-γ, human RXR-α, human PPAR-α, human PPAR-β, human PPAR-γ, human P

Coactivator proteins can be expressed using techniques known in the art, particularly members of the p160 family of coactivator proteins that have been cloned and/or expressed previously, such as SRC-1, AIB1, RAC3, p/CIP, and GRIP1 and its homologues TIF 2 and NcoA-2. A preferred method for expression of coactivator protein is to express a fragment that retains transcriptional activation activity using the "yeast 2-hybrid" method as described by Hong et al. (PNAS supra; and MCB supra), for GRIP1 expression, which reference is herein incorporated by reference

The proteins can be expressed alone, as fragments of the mature or full-length sequence, or as fusions to heterologous sequences. For example, TR can be expressed without any portion of the DBD or amino-terminal domain. Portions of the DBD or amino-terminus can be included if further structural information with amino acids adjacent the LBD is desired. Generally, for the TR the LBD used for crystals will be less than 300 amino acids in length. Preferably, the TR LBD will be at least 150 amino acids in length, more preferably at least 200 amino acids in length, and most preferably at least 250 amino acids in length. For example the LBD used for crystallization can comprise amino acids spanning from Met 122 to Val 410 of the rat TR-α or Glu 202 to Asp 461 of the human TR-β.

Typically the LBDs are purified to homogeneity for crystallization. Purity of LBDs can be measured with sodium dodecyl sulfate polyacrylamide gel electrophoresis (SDS-PAGE), mass spectrometry (MS) and hydrophobic high performance liquid chromatography (HPLC). The purified LBD for crystallization should be at least 97.5 % pure, preferably at least 99.0% pure, more preferably at least 99.5% pure.

Initially, purification of the unliganded receptor can be obtained by conventional techniques, such as hydrophobic interaction chromatography (HPLC), ion exchange chromatography (HPLC), and heparin affinity chromatography.

To achieve higher purification for improved crystals of nuclear receptors, especially the TR subfamily and TR, the receptors can be ligand-shift-purified using a column that separates the receptor according to charge, such as an ion exchange or hydrophobic interaction column, and then bind the eluted receptor with a ligand, especially an agonist. The ligand induces a change in the receptor's surface charge such that when re-chromatographed on the same column, ligand-bound receptor is separated from unliganded receptor. Usually saturating concentrations of ligand are used in the column and the protein can be preincubated with the ligand prior to passing it over the

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5 column. The structural studies detailed herein indicate the general applicability of this technique for obtaining super-pure nuclear receptor LBDs for crystallization.

Purification can also be accomplished by use of a purification handle or "tag," such as with at least one histidine amino acid engineered to reside on the end of the protein, such as on the N-terminus, and then using a nickel or cobalt chelation column for purification. (Janknecht et al., *Proc. Natl. Acad. Sci. USA.* (1991) 88:8972-8976) incorporated by reference.

Typically purified LBD, such as TR LBD, is equilibrated at a saturating concentration of ligand at a temperature that preserves the integrity of the protein. Ligand equilibration can be established between 2 and 37°C, although the receptor tends to be more stable in the 2-20°C range. Preferably crystals are made with the hanging drop methods detailed herein. Regulated temperature control is desirable to improve crystal stability and quality. Temperatures between 4 and 25°C are generally used and it is often preferable to test crystallization over a range of temperatures. The crystals are then subjected to vapor diffusion and bombarded with x-rays to obtain x-ray diffraction pattern following standard procedures.

For co-crystallization with a peptide that binds to the coactivator binding site, various concentrations of peptides containing a sequence that binds to a coactivator binding site of a nuclear receptor of interest can be used in microcrystallization trials, and the appropriate peptides selected for further crystallization. Any number of techniques, including those assays described herein can assay peptides for binding to the coactivator binding site of a nuclear receptor of interest. In a preferred embodiment, a NR-box 2 sequence-containing peptide is used for crystallization with TR LBD. A preferred peptide contains a NR-box (SEQ ID NO: 1) LxxLL motif, and suitable flanking sequences necessary for binding and forming complex with coactivator binding site of the nuclear receptor of interest, such as a TR LBD. The binding peptides are then tested in crystallization trials at various concentrations and ratios of concentrations with a nuclear receptor of interest, for example, as described herein and in the Examples. For crystallization trials with TR LBD, the hanging drop vapor diffusion method is preferred. Conditions of pH, solvent and solute components and concentrations and temperature can be adjusted, for instance, as described in the Examples. In the handing drop method, to obtain suitable crystals for x-ray diffraction analysis, seeding of prepared drops with microcrystals of the complex can be used. Collection of structural information can be determined by molecular replacement using the structure of TR LBD determined herein or previously by Wagner et al., supra. The structure is refined following standard techniques known in the art.

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There are many uses and advantages provided by the present invention. For example, the methods and compositions described herein are useful for identifying peptides, peptidomimetics or small natural or synthetic organic molecules that modulate nuclear receptor activity. The compounds are useful in treating nuclear receptor-based disorders. Methods and compositions of the invention also find use in characterizing structure/function relationships of natural and synthetic coactivator compounds.

The following examples illustrate various aspects of this invention. These examples do not limit the scope of this invention.

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5 **EXAMPLES**

Example 1: Expression and purification of wild-type and mutant nuclear receptors and coactivators

A. Human TRβ LBD

Human TRB LBD (His6-E202-D461) was expressed and purified as described (Shiau et al., Gene (1996) 179(2):205-10). Briefly, the protein was expressed from pET (e.g., pET3 and pET28) in BL21DE3 at 14°C, induced at OD(600nm) 0.7 with 1mM IPTG and incubation was extended for 24 hours. Cells were harvested and lysed in 50mM sodium-phosphate buffer (pH 8.0), 0.3M NaCl, 10% glycerol, 25mM β-merceptoethanol and 0.1mM PMSF as described above. The lysate was cleared by ultracentrifugation (Ti45, 36000 rpm, 1h, 4°C), loaded on a Talon column equilibrated in the sodium phosphate buffer described above, washed with 12mM imidazole and eluted with an imidazole gradient (12 - 300 mM). TRß LBD containing fractions were loaded in 0.6M ammonium sulfate on a TSK-phenyl hydrophobic interaction column and eluted with a reverse ammonium sulfate gradient [0.6 - 0 M] in 50% glycerol and 10% acetonitrile. Fractions containing TRB LBD were tested for hormone binding, pooled and incubated with a 3-fold molar excess of T₃ (Sigma). The hydrophobic interaction run was repeated with liganded receptor under the same conditions. Liganded receptor, which elutes earlier than unliganded receptor, was collected and buffer changed to 20mM Hepes pH7.0, 3mM DTT and 0.1 µM T3 using NAP columns (Pharmacia). For crystallization, the protein was concentrated by ultrafiltration (Millipore UFV2BGC10 concentrators) to a final concentration of 9mg/ml. The yield was about 9.5mg protein per liter bacterial culture.

B. Human TR mutants

Thirty-seven thyroid receptor mutants were created by synthesizing double-stranded oligonucleotides which encode the mutant sequence and which have ends allowing them to be ligated as a cassette using pairs of the Nsil, Pstl, Sstl, AlwNI, Apol, PflMI, BstXI, BseRI, BsmFI, PvuII, NspI, SmaI, PmII, BglII and BsmI restriction sites of the hTR β 1 cDNA sequence, or the 3' plasmid polylinker Sall, or BamHI restriction sites. The hTR β 1 sequences thus mutated were subcloned into the pCMX vector encoding the full-length 461 amino acid hTR β 1 sequence. Some of the mutations of the hTR β 1 in the CMX vector and all three mutations of the hER α in the pSG5-ER-HEGO vector (Tora et al., *EMBO* (1989) 8:1981) were created using Quick Change Site-Directed Mutagenesis Kits (Stratagene). The mutated sequences were verified by DNA sequencing using Sequenase Kits (Stratagene).

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C. Human ERα LBD

The human ER α -LBD 297-554 was overexpressed as described previously (Seielstad, et al., <u>supra</u>) in BL21(DE3)pLysS cells transformed with a modified pET-23d-ERG vector that contained the sequence Met-Asp-Pro fused to residues 297 to 554 of the hER α (provided by Paul Sigler of Yale University). Clarified bacterial lysates were adjusted to 3 M in urea and 0.7 M in NaCl and then applied to a 10-ml column of estradiol-Sepharose (Greene, et al., *Proc. Natl. Acad. Sci. USA* (1980) 77:5115-5119; Landel, et al., *Mol. Endocrinol.* (1994) 8:1407-1419; Landel, et al., *J. Steroid Biochem. Molec. Biol.* (1997) 63:59-73).

To carboxymethylate the solvent-accessible cysteines, the bound hERα-LBD was treated with 5 mM iodoacetic acid in 10 mM Tris, pH 8.1, 250 mM NaSCN (Hegy, et al., *Steroids* (1996) 61:367-373). Protein was eluted with 3 x 10-5 M ligand (either DES or OHT) in 30-100 ml of 50 mM Tris, 1 mM EDTA, 1 mM DTT and 250 mM NaSCN, pH 8.5. The yield of hERα-LBD was typically close to 100% (Seielstad, et al., *Biochemistry* (1995) 34:12605-12615). The affinity-purified material was concentrated and exchanged into 20 mM Tris, 1 mM EDTA, 4 mM DTT, pH 8.1 by ultrafiltration. The protein was bound to a Resource Q column (Pharmacia) and then eluted with a linear gradient of 25-350 mM NaCl in 20 mM Tris, pH 8.1, 1 mM DTT. The hERα-LBD-ligand complexes eluted at 150-200 mM NaCl. Pooled fractions were concentrated by ultrafiltration and analyzed by SDS-PAGE, native PAGE, and electrospray ionization mass spectrometry.

D. Human ER mutants

To test the importance of the NR box peptide/LBD interface observed in the crystal, a series of site-directed mutations were introduced into the ERα LBD. These mutations were designed either to simultaneously perturb the structural integrity and the nonpolar character of the floor of the binding groove (Ile 358->Arg, Val 376->Arg and Leu 539->Arg) or to prevent the formation of the capping interactions (Lys 362->Ala and Glu 542->Lys). Fusions of glutathione-S-transferase (GST) to the wild-type and mutant LBDs were analyzed for their ability to bind ³⁵S-labeled GRIP1 in the absence of ligand or in the presence of DES or OHT.

³⁵S-labeled GRIP1 was incubated with either immobilized GST, immobilized wild type GST-hERα LBD, or immobilized mutant GST-LBDs in the absence of ligand or in the presence of DES or OHT. The bound GRIP1 was quantitated after SDS-PAGE. 1358R, mutant LBD containing a Ile->Arg substitution at residue 358; K362A, mutant LBD containing a Lys->Ala substitution at residue 362; V376R, mutant LBD containing a Val->Arg substitution at residue 376;

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5 L539R, mutant LBD containing a Leu->Arg substitution at residue 539; E542K, mutant LBD containing a Glu->Lvs substitution at residue 542.

In the absence of ligand or in the presence of OHT, fusions to the wild-type protein and all of the mutant LBDs showed no detectable binding to GRIP1. The Ile 358->Arg, Val 376->Arg and Leu 539->Arg mutants were all unable to interact with coactivator in the presence of agonist, confirming the importance of the packing interactions observed in the crystal. Disruption of either the N- or C-terminal capping interaction also compromised GRIP1 binding in the presence of agonist. Only the wild-type GST-LBD was able to recognize the coactivator in the presence of DES.

E. Human ER LBD-GST Fusion Protein

A fusion between glutathione-S-transferase (GST) and amino acids 282-595 of hERα was constructed by subcloning the EcoRI fragment from pSG5 ERα-LBD (Lopez et al., submitted manuscript) into pGEX-3X (Pharmacia). The Ile 358-> Arg, Lys 362->Ala, and Leu 539->Arg mutations were introduced into the GST-LBD construct using the QuikChange Kit (Stratagene) according to the manufacturer's instructions. The Val 376->Arg and Glu 542->Lys mutations were created in the GST-LBD construct by subcloning the Bsml/HindIII fragments of derivatives of pSG5-ER-HEGO (Tora, et al., *supra*) into which these mutations had already been introduced. All constructs were verified by automated sequencing (University of Chicago Cancer Research Center DNA Sequencing Facility).

F. Radiolabeled full-length receptors and coactivator proteins

Wild-type (WT) or mutant pCMV-hTRβ1 vector and the pSG5-GRIP1 and pCMX-SRC-1a vectors were used to produce radiolabeled full-length receptors and coactivator proteins using the TNT coupled Reticulocyte Lysate System (Promega) and [35 S]-Met (DuPont). GST-GRIP1 (amino acids 721-1221), GST-GRIP1 (amino acids 563-1121), GST-SRC-1a (amino acids 381-882), GST-hTRβ1 (full-length, WT or mutants, WT provided by. C. Costa), and the GST-hRXRα (full-length provided by. C. Costa), fusion proteins were produced in *E. coli* strain HB101 as per the manufacturer's protocol (Pharmacia Biotech).

G. Coactivator GRIP1 563-767 His6 GST fusion protein

GRIP1 563-767 was cloned as a Bam HI-Xho I fragment derived from pGEX-2TK GRIP1
563-1121 into the corresponding sites of pGEX-4T1. A His6-tag was added by inserting a Xho I35 Nae I fragment of pET23a into Xho I-Bsa AI sites of this pGEX-4T1 construct yielding pGEX

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GRIP1 563-767His6. Mutants of GRIP1 563-767 were generated by PCR or single stranded mutagenesis using oligonucleotides carrying the mutations and a pSG5 GRIP1 vector as template. The mutations were confirmed by sequence analysis and integrated into pGEX GRIP1 563-767His6 as NgoMI - Xho I fragments. The GRIP1 563-767 His6 GST fusion protein was expressed in HB101 at 37°C. Protein expression was induced with 1mM IPTG at an optical density (600 nm) of 0.7 and extended for 4 hours after induction. Cells were harvested by centrifugation, resuspended in sonication buffer (20mM TrisHCl pH 8.0, 0.1M NaCl, 10%glycerol, 0.1mM PMSF and protease inhibitors (Complete, EDTA free, Boehringer Mannheim)). The resuspended cells were freezethawed once, incubated on ice with 0.1mg/ml lysozyme for 20 minutes and lysed per sonication. The lysate was cleared by ultracentrifugation (Ti 45, 36000rpm, 1h 4°C), the supernatant filtered (Costar 0.2µm top filter) and loaded on a Talon column (Clontech). The column was washed with 10 column volumes of sonication buffer supplemented with 12mM imidazole and eluted with an imidazole gradient [12 - 100mM]. At this step the fusion proteins are about 95% pure. Imidazole was removed by gelfiltration on NAP columns (Pharmacia), and protein concentrations determined using the Biorad protein assay. Equal concentrations of the different derivatives of the fusion fragment were incubated with glutathione agarose (1h, 4°C) which was equilibrated in binding buffer (sonication buffer supplemented with 1mM DTT, 1mM EDTA and 0.01% NP-40). Beads were washed with at least 20 volumes of this buffer, diluted in binding buffer with 20% glycerol to 40%, frozen in aliqots and stored at -70°C.

H. Coactivator GRIP1 563-767 His6

GRIP1 563-767 was cloned as a Bam HI - Xho I fragment derived fron pGEX GRIP1 563-767His6 into corresponding cloning sites of pET23a yielding pETGRIP1 563-767His6. The fragment was expressed in BL21DE3. Expression, cell lysis and Talon purification was identical as described for GST GRIP1 563-767His6. The protein eluted from a Talon column in two fractions, one at 12mM and one between 40 and 70mM imidazole. In the earlier eluting fraction the fragment was associated with a 70 kDa protein which was removed by a MonoQ run in 50mM TrisHCl pH7.5, 10% glycerol, 1mM EDTA, 1mM DTT, 0.1mM PMSF and protease inhibitors. GRIP1 563-767His6 eluted in the flow through and was concentrated by ultrafiltration. At this step the protein was more than 95% pure.

Example 2: Peptide synthesis

Coactivator peptides were obtained using standard techniques. All peptides were HPLC purified and analyzed by mass spectroscopy. Peptide concentrations were either determined

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5 spectroscopically using the tyrosine signal (A₂₇₆ = 1450 M-1cm-1) or by amino acid analysis following standard techniques.

Example 3: Binding assays with nuclear receptors and coactivators

A. GST-GRIP Pull-down Assays and Peptide Competition Assays

Binding experiments were performed by mixing glutathione beads containing 10 μ g of GST fusion proteins (Coomassie Plus Protein Assay Reagent, Pierce) with 1-2 μ l of the [15 S]-labeled wild-type or mutant hTR β 1 (25 fmoles, 4000 cpm of receptor), or coactivators in 150 μ l of binding buffer (20 mM HEPES, 150 mM KCl, 25 mM MgCl₂, 10% glycerol, 1 mM dithiothreitol, 0.2 mM phenylmethylsulfonyl fluoride, and protease inhibitors) containing 2 mg/ml BSA for 1.5 hrs in the presence or absence of 1 μ M T₃. Beads were washed 3 times with 1 ml of binding buffer and the bound proteins were separated using 10% SDS-PAGE and visualized by autoradiography. Binding was quantitated by phosphorimaging using ImageQuant (Molecular Dynamics).

For in vitro binding studies GR, TR and their derivatives were translated in the presence of [35S]methionine using the TNT Coupled Reticulocyte System (Promega). Separate translations were performed in the presence and absence of $10\mu M$ dexamethasone or $1\mu M$ RU486 for GR and $10\mu M$ triiodothyronine for TR. Expression was quantified by phosphoimager analysis (BAS2000, Fuji). For all binding assays 50µl of a 20% bead suspension containing either 1.6 or 4.0 µM bound purified GST GRIP1 fragment (either 568-767 or 563-1121) was incubated with 0.2µl or 1.4µl in vitro transcribed and translated TR or GR, respectively. Binding was performed in the binding buffer described above supplemented with 20 µg/ml BSA and appropriate hormone. The chosen GST GRIP1 fragment concentrations were sufficient to bind either 70 or 100% of the TR derivatives. The reaction was incubated at 4°C under rotation for 2 hours. In case of competition experiments, the appropriate concentration of peptides were added to the reaction before addition of receptors. However, no differences in the results were noted by adding the peptides after half of the incubation of the GST GRIP1 fragment with nuclear receptors. This demonstrates that equilibrium is reached under the chosen conditions. Beads were washed five times with 200µl binding buffer + BSA at 4°C before elution of the bound proteins in 20µl SDS loading buffer. Eluted beads and input labeled protein were subjected to SDS-PAGE. The fraction of bound nuclear receptors was determined by phosphoimager analysis.

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B. GST-hTRβ1 Pull-down Assays

Assay and analysis was performed as for Example 3A. *In vitro* binding of [³⁵S]-labeled full-length GRIP1, [³⁵S]-labeled full-length SRC-1a, and [³⁵S]-labeled full-length hRXRα, to GST-hTRβ1 wild-type (WT) and mutants was performed. Mutants V284R, K288A, I302R, L454R, and E457K all bound to hRXRα with an affinity equivalent to wild type hTR. All of these mutants showed decreased ability to bind GRIP1 and SRC-1a, as expected from the results of Example 3A. The same results were obtained when a GST-SRC1 construct including SRC-1a amino acids 381-882 was tested for binding of [³⁵S]-Met-labeled full-length hTRβ1 WT and mutants (data not shown).

C. GST-hERa LBD Pull-down Assays

The wild-type and mutant GST-hERα LBDs were expressed in BL21(DE3) cells. Total ligand binding activity was determined by a controlled pore glass bead assay (Greene, et al., *Mol. Endocrinol.* (1988) 2:714-726) and protein levels were monitored by western blotting with a monoclonal antibody to hERα (H222). Cleared extracts containing the GST- hERα LBDs were incubated in buffer alone (50 mM Tris, pH 7.4, 150 mM NaCl, 2 mM EDTA, 1 mM DTT, 0.5% NP-40 and a protease inhibitor cocktail) or with 1 μM of either DES or OHT for 1 hour at 4°C. Extract samples containing thirty pmol of GST-LBD were then incubated with 10 μl glutathione-Sepharose-4B beads (Pharmacia) for 1 hour at 4°C. Beads were washed five times with 20 mM HEPES, pH 7.4, 400 mM NaCl, and 0.05% NP-40. ³⁵S-labeled GRIP1 was synthesized by *in vitro* transcription and translation using the TNT Coupled Reticulocyte Lysate System (Promega) according to the manufacturer's instructions and pSG5-GRIP1 as the template. Immobilized GST-hERα LBDs were incubated for 2.5 hours with 2.5 μl aliquots of crude translation reaction mixture diluted in 300 μl of Tris-buffered saline (TBS). After five washes in TBS containing 0.05% NP-40, proteins were eluted by boiling the beads for 10 minutes in sample buffer. Bound ³⁵S-GRIP1 was quantitated by fluorography following SDS-PAGE.

D. Electrophoretic Mobility Shift Assays

GRIP1, a mouse p160 coactivator, recognizes the ER α LBD in a ligand-dependent manner. The binding of agonists to the ER α LBD promotes recruitment of GRIP1, whereas binding of antagonists prevents this interaction (Norris, et al., *J. Biol. Chem.* (1998) 273:6679-88). While

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5 agonist-bound receptor will bind to all three of the NR boxes from GRIP1, ERα strongly prefers NR-box 2 (Ding, et al., Mol. Endocrinol. (1998) 12:302-13).

An electrophoretic mobility shift assay was used to directly assess the ability of the NR-box 2 peptide to bind the purified ER α LBD in the presence of either DES or OHT. Eight microgram samples of purified hER α -LBD bound to either DES or OHT were incubated in the absence of the peptide, i.e., buffer alone, or in the presence of either a 2-fold or 10-fold molar excess of the GRIP1 NR-box 2 peptide. The binding reactions were performed on ice for 45 minutes in 10 μ l of buffer containing 20mM Tris, pH 8.1, 1mM DTT, and 200mM NaCl and then subjected to 6% native PAGE. Gels were stained with GELCODE Blue Stain reagent (Pierce).

In the presence of the NR-box 2 peptide, the migration of the DES-hERα-LBD complex was retarded. In contrast, peptide addition had no effect on the mobility of the OHT-hERα-LBD complex. Hence, this peptide fragment of GRIP1 possesses the ligand-dependent receptor binding activity characteristic of the full-length protein.

Example: 4 Transfection assays with TR and hER α

HeLa cell transfection and assay conditions are described (Webb et al., *Mol Endocrinol* (1995) 9:443). For TR assays, 5 μ g of the reporter p(DR-4)₂ -TK-LUC consisting of two copies of the DR-4 element (a direct repeat of the consensus TR response element (TRE) spaced by 4 base pairs) placed upstream of a minimal (-32/+45) thymidine kinase gene promoter linked to luciferase (LUC) coding sequences were used. A reporter containing palindromic TREs gave the same results (data not shown). Also, 2 μ g of the hTR β 1 expression vector, pCMX-TR (WT or mutant), and 0.5 μ g transfection control vector, pJ3LacZ, which contains the SV40 promoter linked to the β -galactosidase gene, were used. Other cells co-transfected with vector or receptor constructs can be used for same purpose. Alternative cells expressing sufficient levels of an endogenous receptor(s), or cells selected that express a single reporter, can be used for transfection assays, including MCF-7 cells expressing ER (Webb et al., \underline{supra}), and GC cells expressing TR (Norman et al., J. Biol. Chem. (1989) 264:12063-12073).

For hER α assays, 5 μ g of estrogen responsive reporter plasmid encoding chloramphenicol acetyltransferase (CAT), pERE-collTATA (Sadovsky, et al., Mol Cell Biol. (1995) 15:1554), 0.5 μ g expression vector encoding full-length hER α , pSG5-er HEGO (WT or mutants), and 2 μ g of pj3lacz, were used. For the experiments of **Figures 2** and **4**, 0.5 μ g of a full-length GRIP1 expression vector, pSG5-GRIP1, was also included in the transfection. Transfected cells were

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5 treated with or without 1 μM T₃ or E₂, as indicated. After culturing for 24 hrs, the LUC or CAT activities were assayed and the β-galactosidase activities were also assayed to correct for differences in transfection efficiencies. The triplicate points were averaged and standard deviations were less than 10%.

Example 5: Hormone binding assays for wild-type and mutant TRs

The T₃ binding affinity constants (Kd) for *in vitro* -translated WT and mutant TRs were measured using $[^{125}I]$ 3,5,3' triiodo-L-thyronine ($[^{125}I]$ T₃) in gel filtration binding assays as described (Apriletti et al., *Protein Expr. Purif.* (1995) 6:363). Both the Kd and standard error (S.E.) values were calculated using the Prism computer program (GraphPad Software, Inc.). Mutations are indicated by the single-letter amino acid abbreviations, with the native residue name, followed by the primary sequence position number, and then the mutated residue name. The affinity of the WT TR is 81 ± 12 pM. The relative affinity was determined by dividing the WT Kd by each mutant Kd. The 37 mutants tested with their relative affinities are: E217R (123%), E227R (109%), K242E (92%), E267R (117%), H271R (123%), T277R (7%), T281R (145%), V284R (105%), D285A (89%), K288A (98%), C294K (94%), E295R (118%), C298A (87%), C298R (141%), E299A (171%), I302A (86%), I302R (99%), K306A (6%), K306E (6%), P384R (164%), A387R (107%), E390R (151%), E393R (146%), L400R (95%), H413R (109%), H416R (153%), M423R (156%), R429A (48%), S437R (170%), L440R (174%), V444R (89%), T448R (234%), E449R (36%), P453E (32%), L454R (26%), L456R (46%), E457K (71%).

Example 6: Coactivator binding assays for wild-type and mutant TRs

Wild type (WT) TR and most of the TR mutants liganded to 3,5,3'-triiodo-L-thyronine (T₃) bind equally well to the coactivator, GRIP1. In all cases, GRIP1 binding was hormone-dependent (data not shown). Mutations L454R and E457K in surface residues of helix 12 abolish GRIP1 binding (Figure 1). Mutations in two residues of helix 3, V284R and K288A, and two residues of helix 5, I302R and K306A, also impair binding (Figure 1). Five mutations with diminished GRIP1 binding (V284R, K288A, I302R, L454R, and E457K) also show decreased binding to another coactivator, SRC-1a (data not shown). Thus, these results show that two different coactivators recognize the same TR surface residues.

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5 Example 7: TR residues involved in ligand-dependent transcription activation in context of a cell

Residues involved in ligand-mediated transcription activation were identified by testing the TR mutants of Example 8 in HeLa cells. T₃ increased reporter gene activity 5-fold in cells expressing either WT TR or mutated TRs showing normal GRIP1 binding (representative mutants are shown in Figure 1. By contrast, TR mutants with diminished or absent GRIP1 binding (V284R, K288A, I302R, K306A, L454R, and E457K) show a diminished or absent response to T₃ which correlates with the GRIP1 binding defect. Overexpression of GRIP1 increases activation by the WT TR and rescues activation by TR mutants roughly in proportion to the severity of the defect of GRIP1 binding and activation (Figure 2). These results suggest that the same residues are required for coactivator binding, function of the endogenous coactivator(s) in HeLa cells, and responsiveness of TRs to GRIP1.

Example 8: Effect of TR mutations on other receptor functions

The effects of the mutations on other receptor functions also were examined. All of the mutants bound radiolabeled thyroid hormone (Kd values, 6%-234% that for native receptor); occasional lower values were expected because some residues have partially buried side chains. None of the residues that decrease GRIP1 binding affected TR binding to a GST-RXR fusion protein or to DNA using three different DNA half-site arrangements and testing with or without added RXR (data not shown). Some mutations that affect GRIP1 binding occur in a region spanning helices 3-5, which has been suggested as important for TR/RXR heterodimerization (O'Donnell et al., supra; Lee et al., Mol. Endocrinol. (1992) 6:1867-1873). In contrast, however, the above results indicate that these residues do not contribute to TR/RXR heterodimerization. Further, TRs mutated in the CBS residues retain the ability of WT TR of T3-dependent inhibition of the activity of the Jun and Fos transcription factors at an AP-1 site (Saatcioglu et al., supra), suggesting that the CBS residues do not participate in TR actions mediated through these proteins. These data indicate that the mutational effects are specific, the amount of input labeled TR in the different reactions is comparable, and the levels of expression of the mutant TRs are comparable to those of WT receptors.

Example 9: Coactivator binding site in ER

Three separate mutations (K362A, V376R, and E542K) were created in human estrogen receptor- α (hER α) which align to three of the effective positions in hTR β 1 (K288A, I302R, and

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5 E457K). All three mutations diminish GRIP1 binding and abolish transcriptional activation (Figure 3), and mutant V376R, with 10% residual GRIP1 binding, was rescued partially by overexpression of GRIP1 (Figure 4). As a control, the ER mutants demonstrated a normal hormone-dependent ability to activate a vitellogenin-LUC hybrid reporter gene, GL45, which responds to the ER amino-terminal activation function (Berry et al., EMBO J (1990) 9:2811-2818)
10 (data not shown). The finding that similar residues are required for GRIP1 binding and transcription activation activity in the TR and ER suggests that the coactivator binding site residues are similar in different nuclear receptors.

Example 10: Coactivator NR-box binding affinity for TR

To study the interaction between nuclear receptors and GRIP1 in vitro, a fragment of GRIP1 (563-767) was purified that contains all three NR-boxes (Figures 6 and 7). The fragment was found to be highly soluble and, in agreement with a secondary structure prediction using PhD, displays a mainly alpha-helical far UV-CD spectrum (data not shown). Three of the four helices predicted for the fragment include the NR-boxes at their C-terminus, suggesting that these boxes are part of amphipathic alpha-helices. These results show that the NR-boxes of GRIP1 are contained in a soluble, alpha-helical 24kD fragment.

Binding assays show that GRIP1 NR-boxes 1, 2 and 3, interact differentially with hTRß LBD (Figure 7). A GST-fusion of the GRIP1 (563-767) fragment strongly binds TR (kD or EC50) in a ligand depend fashion. Replacement of the hydrophobic residues of NR-box 3 with alanine does not reduce binding of TR significantly, whereas similar replacement of NR-box 2 results in loss of TR binding of about 50%. By titrating the amount of GRIP1 fragment, about a 4-fold stronger binding of TR for NR-box 2 (EC50 = 1.0 µM) over NR-box 3 (EC50 = 4.0 µM) was estimated. In the absence of functional NR-boxes 2 and 3, almost no binding to TR was detected suggesting that under these experimental conditions NR-box 1 is not a cognate binding site for TR. Full length TR or TR-LBD bound GRIP1 equally. These results show that TR recognizes GRIP1 NR-box 2 and 3, with preference for NR-box 2.

Example 11: Coactivator NR-box binding affinity for GR

GR also was found to bind GRIP1 (563-767) in a ligand-dependent manner (Figure 8). However, in contrast to TR, extension of GRIP1 (563-767) to residue 1121 increases binding to GR about 3-fold suggesting an additional binding site on GRIP1 for GR. Binding of the larger fragment remains ligand-dependent; no interaction can be observed in the presence of the GR partial

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antagonist RU486. These results are in agreement with in vivo 2-hybrid GR GRIP1 interaction studies. In the presence of ligand no difference was detected in the binding of GRIP1 by full length GR or a deletion mutant of GR that lacks the N-terminal activation domain AF-1. However in the absence of ligand, binding of GR to GRIP1 (563-1121) increased by about 10-fold indicating that sequences in the GR N-terminus are able to suppress binding of unliganded GR to this additional binding site in GRIP1. Additionally, GR did not bind to a GRIP1 (563-767) mutant in which both NR-box 2 and 3 are replaced by alanines, and binds most strongly to a fragment that lacks a functional NR-box 2. As with TR, GR does not recognize NR-box 1. In contrast to TR, the GR prefers NR-box 3 to NR-box 2. These results demonstrate that GR prefers binding to NR-box 3 and interacts with an additional GRIP1 site within the CREB (cAMP - response - element binding protein) - binding protein (CBP) binding site.

Example 12: Coactivator peptide binding affinity for TR

To investigate whether the preference of TR for NR-box 2 is dependent on the sequence or structural context of the NR-boxes, competition studies on the interaction of GRIP1 with hTRß LBD were performed using coactivator peptides containing different NR- boxes (NR-box 2 peptide (residues 11-23 of SEQ ID NO: 6) EKHKILHRLLQDS, and NR-box 3 peptide (residues 9-21 of SEQ ID NO: 7) ENALLRYLLDKDD) (**Figure 9**). Consistent with the interaction of hTR LBDß with GRIP1 (563-767) NR-box mutants, a peptide containing NR-box 1 competes the interaction of GRIP1 with hTRß LBD only at very high concentrations (EC50 = 130 μ M). Peptides containing either NR-box 2 or 3 compete GRIP1 (563-767) efficiently and display the preference of hTRß LBD for NR-box 2 (EC50 (NR-box 2) = 1.5 μ M, EC50 (NR-box 3) = 4 μ M). The apparent affinities (EC50) for peptides of NR-box 2 and 3 are comparable with the analogous GRIP1 (563-767) NR-box mutants suggesting that the preference of TR for NR-boxes is solely dependent on the sequence and independent of the structural context of the NR-boxes.

Peptides of NR-box 2 or 3 compete GRIP1 (563-767) containing functional NR-boxes 2 and 3 or a mutant of this fragment that contains only a functional NR-box 2 with comparable affinity. Thus, while TR can bind both NR-box 2 and 3, in a GRIP1 coactivator peptide fragment containing both boxes. TR preferentially binds NR-box 2.

These results show the preference of TR for NR-box 2 is sequence dependent.

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The same types of assays for TR competition are performed to assess coactivator peptide binding affinity for GR. The peptide concentrations are normalized relative to TR for obtaining comparable dose response curves.

Example 13: Binding affinity of TR for extended coactivator peptides

Sequence identity between all three central NR-boxes of the p160 coactivator family is limited to the conserved leucine residues of the (SEQ ID NO: 1) LxxLL motif (Figure 6). However, the sequence conservation of a particular NR-box can extend into neighboring residues. To investigate the contribution of these neighboring residues to affinity and specificity of the different NR-boxes for TR, the ability of peptides containing individual NR-boxes with different lengths of adjacent sequences to compete with the interaction of GRIP1 (563-767) with hTRB LBD were compared (Figure 10).

A peptide consisting of the minimal motif of NR-box 3 (residues 12-17 of SEQ ID NO: 7; LLRYLL) does not compete the TR LBD interaction with GRIP1 (563-767). A peptide consisting of the NR-box 2 (residues 15-20 of SEQ ID NO: 6; ILHRLL) also does not sufficiently compete the interaction (data not shown). Extending peptides containing a (SEQ ID NO: 1) LxxLL motif to include adjacent residues increased affinity for both NR-box motifs and magnified the preference of TR for NR-box 2 (NR-box 2 peptides: (residues 11-23 SEQ ID NO: 6) EKHKILHRLLQDS and (residues 7-23 of SEQ ID NO: 6) TSLKEKHKILHRLLQDS; and NR-box 3 peptides: (residues 8-24 of SEQ ID NO: 7) KENALLRYLLDKDDTKD and (residues 5-24 of SEQ ID NO: 7) PKKKENALLRYLLDKDDTKD). A chimeric peptide containing the NR-box 3 motif in the context of the NR-box 2 flanking sequences (SEQ ID NO: 31; TSLKEKHKLLRYLLQDSS) binds like a NR-box 2 peptide.

These results demonstrates that preference of TR for NR-box 2 is at least partially due to features of the bound peptide (residues 15-20 of SEQ ID NO: 6; ILHRLL), but that their affinity and specificity is modulated by adjacent sequences.

30 Example 14: Binding affinity of TR and GR for mutant coactivator

A. TR affinity for ILxxLL motif residues

To investigate the role of the hydrophobic residues in NR-box 2, individual residues of the (residues 15-20 of SEQ ID NO: 6) ILHRLL motif were replaced by alanine in the background of GRIP1 (563-767) containing a non-functional NR-box 3 (Figure 11). Surprisingly, replacement of

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any of the conserved leucines prevents binding to TR almost completely. Only replacement of the nonconserved isoleucine exhibited a lessened but still severe impact on the affinity of NR-box 2 for TR. As replacement of a single leucine by alanine is sufficient to overcome the interaction of both the remaining hydrophobic residues and adjacent sequences with hTRB LBD, it appears that their contribution to the affinity of NR-box 2 for hTRB LBD is cooperative rather than additive.

Similar results were obtained by competing the interaction of hTRB LBD with the GRIP1 (563-767) NR-box 3 mutant using peptides in which either IL, HR or LL of the NR-box 2 motif are replaced by alanines (Figure 11). Whereas the peptides containing the IL or LL replacement failed to interact with the hTRB LBD even at very high concentrations, in agreement with a proposed alpha-helical structure of the motif, replacement of the "HR spacer" by alanines showed a marginal effect on the affinity of the peptide for TR-LBD.

Replacement of single leucine residues of NR-box 2 by phenylalanine reduced the affinity of NR-box 2 peptides for TR LBD about 100-fold, replacement of the isoleucine about 10-fold (Figure 11). Therefore, the interaction of TR with GRIP1 relies not simply on the hydrophobicity of the (SEQ ID NO: 1) LxxLL motif, but also on positive contributions by the leucine residues themselves.

These results demonstrate that single mutations of the conserved leucines in the (SEQ ID NO: 1) LxxLL motif strongly reduce affinity of GRIP1 for hTRB LBD.

Collectively, the above examples demonstrate that peptides containing NR-boxes, particularly NR-box 2, reproduce the affinity and specificity of the interaction of GRIP1 (563-767) with hTRB LBD.

B. TR affinity of FxxLW and FxxAL motif residues

The three conserved leucines of the NR-box 2 (SEQ ID NO: 2) ILxxLL motif are embedded in the hydrophobic cleft of the hTRB LBD:NR-box 2 interaction surface, whereas the non conserved isoleucine is located on the rim of this cleft where structural changes can be more easily accommodated (See Example 18). In agreement with this structure, replacement of this residue by alanine or phenylalanine reduced binding to hTRB LBD to a less extent than the comparable mutations of the conserved leucine residues. The surface generated by the three conserved leucines (L690, L693, L694) of the NR-box 2 peptide (residues 12-24 of SEQ ID NO: 6) 686-KHKILHRLLQDSS-698 is highly complementary to the corresponding binding site in the hTRB LBD (Figures 16 and 17). Comparison of this binding site to other nuclear receptors shows that it

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contains a structural motif that is unique, highly conserved and present in all known structures of nuclear receptor LBDs (Wurtz et al., *Nat Struct Biol.* (1996) 3:87-94; Wagner et al., *supra*; Renaud et al., *Nature* (1995) 378:681-689; Bourguet et al., *Nature* (1995) 375:377-382; and Brzozowski et al., *Nature* (1997) 389:753-758).

Interaction of highly conserved hydrophobic motifs, which are part of amphipathic alphahelices, with complementary hydrophobic surfaces resembles a feature observed for the interaction of several other transcriptional activators with their target proteins (p53:MDM2, VP16:TAFII31 or CREB:KIX-CBP). However, the motifs of p53 (FxxLW), VP16 (FxxAL) and CREB (YxxIL) differ from the (SEQ ID NO: 1) LxxLL motif of nuclear receptor coactivators. A Fxxxh motif may be generally involved in interaction with TAFII31, where "h" represents any hydrophobic residue. Though with respect to the known structures, complementarity of the interacting hydrophobic surfaces identified here seem to be a common feature of these interactions, cross-reactions between different motifs are possible. For instance, VP16, p53, and p65 (FxxFL) are able to functionally interact with TAFII31, or p53 and E2F1-DP1 (FxxLL) both interact with MDM2. These interactions are sensitive to mutations in the Fxxxh motif. Therefore it appears that either complementarity of the hydrophobic surfaces is not an absolute requirement or that induced fitting of the interacting surfaces is possible.

Based on these observations, studies were performed to determine whether GRIP1 interacts with TAFII31 or MDM2. However, no interaction was detected. GRIP1 mutants changing NR-box 2 (SEQ ID NO: 1; LxxLL) to VP16 (SEQ ID NO: 4; FxxAL) or p53 (SEQ ID NO: 3; FxxLW) like binding sites also failed to bind TAFII31 or MDM2 demonstrating that the presence of the correct binding site is not sufficient to create binding (data not shown). Moreover, peptides containing the VP16 or p53 binding sites are not able to compete the interaction of GRIP1 with TR, even in very high concentration, but do compete the interaction with GR (data not shown). The affinity of this interaction is weak, but comparable to affinity of a peptide of NR-box 2 that, in the context of a GRIP1 mutant lacking NR-box 3, binds GR in vivo (Ding et al., supra). This binding is only about ten times less than a peptide containing NR-box 3, GR's primary binding site.

As shown above, GR binds GRIP1 (563-767) with about one-fifth the affinity than a comparable amount of TR. Thus, the high concentration of NR-box 3 peptide required to compete the interaction of GR with GRIP1 (563-767) may rather reflect a weak affinity of GR for the peptide rather than a particular strong interaction of GR with GRIP1 (563-767).

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These results suggest that at least on the peptide level, other hydrophobic motifs besides (SEQ ID NO: 1) LxxLL can interact with the coactivator binding site, but that it is receptor dependent.

C. TR affinity for residues adjacent to ILxxLL motif

Peptides containing a FxxLL motif bind TR but with two orders of magnitude lower affinity than a (SEQ ID NO: 1) LxxLL motif (Figure 11). To test whether the additional changes in the hydrophobic motif or adjacent sequences of the VP16 peptide prevent its binding to TR, a chimeric peptide containing the NR box-2 motif (SEQ ID NO: 1) LxxLL in the context of the VP16 sequence was constructed. This peptide binds to TR but with an about 100-fold lower affinity than the original NR-box 2 peptide. Thus, the inability to bind the VP16 peptide appears to be due to the combination of an imperfect hydrophobic motif and the incompatibility of TR to adjacent sequences of the VP16 motif.

As the interaction of the chimeric peptide with GR was comparable to the original NR-box 2 and VP16 peptides, this incompatibility appears due to TR-specific features in the NR-box interaction surface. These results show sequences adjacent the NR-box motif LxxLL can reduce binding of NR-box 2 to TR, but not GR.

Example 15: Crystallization and Structure Determination of NR LBD Complexes

A. Crystallization of hTRß LBD with T3 and GRIP1 NR-box 2 Peptide

Several peptides containing GRIP1 NR-box 2 were tested in crystallization trials with the hTRß LBD. The complex of the hTRß LBD with the GRIP1 NR-box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6) produced crystals that were dependent on both the presence and the concentration of the peptide. Without the peptide, the hTRß LBD precipitated immediately. However, nucleation was erratic, but could be overcome through seeding of prepared drops with microcrystals of the hTRß LBD:GRIP1 NR-box 2 peptide complex. Structure of the hTRß LBD:GRIP1 NR-box 2 peptide complex was determined by molecular replacement using the structure of the hTRß LBD determined previously (Wagner et al., *supra*), and refined to a resolution of 3.6Å (Table 1). The refined model consists of residues K211-P254 and V264-D461 of monomer 1 of the hTRß LBD, residues K211-P254 and G261-D461 of monomer 2 of the hTRß LBD, and the GRIP1 NR-box 2 peptides (residues 14-24 of SEQ ID NO: 6) 688-

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5 KILHRLLQDSS-698, and (residues 14-22 of SEQ ID NO: 6) 688-KILHRLLQD-696 (Appendix 1).

Briefly, the complex between the hTRß LBD and the GRIP1 NR-box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6) was prepared by mixing (equal) volumes of a solution of 9mg/ml hTRß LBD in 20mM HEPES pH 7.4 with a solution of 14 mM GRIP1 in 0.4mM ammonium acetate pH 4.72, and incubating the mixture on ice for 1 hour. Crystals were obtained after 2 days at 4°C using hanging drop vapor diffusion from a drop containing 1.5µl of hTRß LBD:GRIP1 complex, prepared as described, and 0.5µl 15%PEG 4K, 0.2M sodium citrate pH 4.9, suspended above a reservoir containing 10% PEG 4K, 0.1M ammonium acetate, and 0.05 M sodium citrate (pH 5.6). After allowing the drop to equilibrate for 1 hour, 0.2µl of 10-3 to 10-5 dilutions of microcrystals in reservoir buffer were introduced to provide nucleation. Crystals are of space group P3121 (a=95.2, b=95.2, c=137.6) and contain two molecules of the hTRß LBD and two molecules of the GRIP1 NR-box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6).

Table 1

Data collection, phasing, and refinement statistics

			Da	ta collection	1		
Data set		olution (Å)	Reflect	tions	Coverage (%)	R _{sym}	
Native		3.6	measured 35565	unique 8490	96.3	0.007	
			Rot	ation searc	h		
Search model	Euler angles (°)				Correlation coefficient		
		Θ_1	Θ_2	Θ ₃	Highest peak	Highest false peal	
hTR β LBD	Ml	60.12	80.68	241.90	16.3		
	M2	9.93	87.70	180.6	15.9	14.2	
			Tran	slation sear	ch		
	Fractional coordinates				Translation function		
		x	у	z	Highest peak (o)	Highest false peak (o	
	Ml	0.522	0.428	0.250	19.52	10.02	
	M2	0.200	0.932	0.119	26.11	5.77	
			F	Refinement			
	Re	solution (Å)	Ref	lection	R	R _{free}	
F > 2(25 - 3.7	70	514	0.2990	0.3219	

 $R_{\text{sym}} = \Sigma_h \Sigma_i \mid I_{h,i} \ \hat{u} \mid (I_h \mid / \Sigma I_h \text{ for the intensity } (I) \text{ of } i \text{ observations of reflection } h.$ Correlation coefficient = $\Sigma_h E \sigma^2 E c^2 - E \sigma^2 E c^2 / [\Sigma_h (E \sigma_2 - E \sigma^2)^2 \Sigma_h (E \sigma^2 - E \sigma^2)^2]^{1/2}$

Translation function $(\mathbf{t}_a, \mathbf{t}_b, \ldots) = \Sigma_h (|Eo_{(b)}|^2 - \Sigma_h \langle |Eo_{(b)}|^2 \rangle) (Ec_{(b, \mathbf{t}_a, \mathbf{t}_b, \ldots)}|^2 - \langle |Ec_{(b)}|^2 \rangle$ where E_0 represents the normalized observed structure factor amplitudes, and E_0 represents the normalized structure factors for the search model in a triclinic unit cell with dimensions identical to that of the crystal. The reported peak height represents the value of the function for the translation $(\mathbf{t}_a, \mathbf{t}_b)$ of the NCS monomers, divided by the rms value of the translation function density.

R factor = $\Sigma | F_{obs} - F_{calc} | / \Sigma | F_{obs} |$.

R_{free} is calculated the same as R factor, except only for 10% of the reflections that were set aside for cross validation and not used in refinement.

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B. Crystallization of hERα LBD with DES and GRIP1 NR-box 2 Peptide

Crystals of a DES-hERa LBD-GRIP1 NR-box 2 peptide complex were obtained by hanging drop vapor diffusion. Prior to crystallization, the DES-hERα LBD (residues 297-554) complex was incubated with a 2-4 fold molar excess of the GRIP1 NR-box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6) for 7-16 hr. Two μL samples of this solution were mixed with equal volume samples of reservoir buffer consisting of 25-27% (w/v) PEG 4000, 90 mM Tris (pH 8.75-9.0) and 180 mM Na Acetate and suspended over wells containing 800 μL of the reservoir buffer. After 4-7 days at 19-21°C, rod-like crystals were obtained. The coactivator complex crystals lie in the spacegroup P2₁ with cell dimensions a=54.09, b=82.22, c=58.04 and β=111.34. Two molecules each of the DES-LBD and the coactivator peptide form the asymmetric unit. A 200 μm x 40 μm x 40 μm crystal was transferred to a cryosolvent solution containing 25% (w/v) PEG 4000, 10% (w/v) ethylene glycol, 100 mM Tris (pH 8.5), 200 mM Na Acetate and 10 μM peptide and frozen in an N2 stream at -170°C in a rayon loop. Diffraction data from this crystal were measured at -170°C using a 300 mm MAR image plate at the Stanford Synchrotron Radiation Laboratory (SSRL) at beamline 7-1 at a wavelength of 1.08 Å. The diffraction images were processed with DENZO and scaled with SCALEPACK (Otwinowski, et al., Methods Enzymol. (1997) 276:307-326) using the default -3σ cutoff.

C. Crystallization of hERa LBD with OHT

Crystals of the hER α LBD (residues 297-554) complexed to OHT were obtained by the hanging drop vapor diffusion method. Equal volume aliquots (2 μ L) of a solution containing 3.9 mg/mL protein-ligand complex and the reservoir solution containing 9% (w/v) PEG 8000, 6% (w/v) ethylene glycol, 50 mM HEPES (pH 6.7) and 200 mM NaCl were mixed and suspended over 800 μ L of the reservoir solution. Hexagonal plate-like crystals formed after 4-7 days at 21-23°C. Both crystal size and quality were improved through microseeding techniques. These crystals belong to the space group P6s22 with cell parameters a=b=58.24 Å and c=277.47 Å. The asymmetric unit consists of a single hER α LBD monomer; the dimer axis lies along a crystallographic two-fold. A single crystal (400 μ m x 250 μ m x 40 μ m) was briefly incubated in a cryoprotectant solution consisting of 10% (w/v) PEG 8000, 25% (w/v) ethylene glycol, 50 mM HEPES (pH 7.0) and 200 mM NaCl and then flash frozen in liquid N2 suspended in a rayon loop. Diffraction data were measured at -170°C using a 345 mm MAR image plate at SSRL at beamline 9-1 and at a wavelength of 0.98 Å. The diffraction images were processed with DENZO and scaled with SCALEPACK (Otwinowski, et al., supra) using the default -3 σ cutoff.

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5 Example 16: Structure determination and refinement of NR LBD complexes

A. Structure of hTRB LBD with T₃ and GRIP1 NR-box 2 Peptide

Data were measured using Cu Ka radiation from an R-axis generator at 50 kV and 300 mA with a 0.3mM collimator and a Ni filter. Reflections were measured using an R-Axis II detector and integrated with Denzo, and equivalent reflections scaled using Scalepack (Otwinowski and Minor, "Processing of x-ray diffraction data collected in oscillation mode." In Macromolecular Crystallography, Part A (ed. C.W. Carter, Jr. and R.M. Sweet), pp. 307-326. Academic Press, New York, NY). Possible rotation function solutions were calculated using normalized amplitudes in AMORE from a model of hTRB LBD with the ligand, T3, omitted; translation function solutions were subsequently determined using TFFC for the two rotation solutions with the highest correlation coefficients. For two hTRB LBD molecules in the asymmetric unit, the calculated solvent content is 52%. After rigid body refinement of the two hTRB LBD molecules, electron density maps were calculated. Strong positive density present in both the anomalous and conventional difference Fourier maps for the iodine atoms of the T3 ligand confirmed the correctness of the solution. The iodine atoms for both T3 ligands were modeled as a rigid body, and the structure refined with strict NCS symmetry using CNS. Both 2FoFc and FoFc electron density maps showed interpretable density, related by the NCS operator, near H12 of both molecules of the hTRß LBD. The electron density could be modeled as a short α-helix, and the observed side chain density was used to tentatively assign the sequence and direction to the chain. The refined model consists of residues of the hTRB LBD, and peptide residues of the GRIP1 NR-box 2 peptide 686-KHKILHRLLODSS-698 (residues 12-24 of SEQ ID NO: 6).

Atomic coordinates of the hTRß LBD:GRP1 site 2 peptide complex are attached as Appendix 1.

B. Structure of hERα LBD with DES and GRIP1 NR-box 2 Peptide

Initial efforts to determine the structure of the DES-hERα LBD-NR box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6) complex utilized a low resolution (3.1 Å) data set (data not shown). A self-rotation search implemented with POLARRFN ("The CCP4 suite: programs for protein crystallography", *Acta Crystallogr*. (1994) D50:760-763) indicated the presence of a noncrystallographic dyad. The two LBDs in the asymmetric were located by molecular replacement in AMoRe (CCP4, 1994) using a partial polyalanine model of the human RARγ LBD (Renaud, et al., *supra*) as the search probe (R=58.2%, CC=35.6% after placement of

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5 both monomers). Given that the model at this point was both inaccurate (r.m.s.d. 1.7 Å between this model and the final model based on Cα positions) and incomplete (accounting for only ~45% of the total scattering matter in the asymmetric unit), an aggressive density modification protocol was undertaken. Iterative cycles of two-fold NCS averaging in DM (CCP4, 1994) interspersed with model building in MOLOC (Muller, et al., Bull. Soc. Chim. Belg. (1988) 97:655-667) and model refinement in REFMAC (Murshudov, et al., Acta Crystallogr. (1997) D53:240-255) (using tight NCS restraints) were used to quickly build a model of the LBD alone. For this procedure, MAMA (Kleywegt, et al., "Halloween...masks and bones. In From First Map to Final Model", Bailey, et al, eds., Warrington, England, SERC Daresbury Laboratory, 1994) was used for all mask manipulations and PHASES (Furey, et al., PA33 Am. Cryst. Assoc. Mtg. Abstr. (1990) 18:73) and the CCP4 suite (CCP4, 1994) were used for the generation of structure factors and the calculation of weights.

However, although the DES-hERα LBD-NR complex model accounted for ~90% of the scattering matter in the asymmetric unit, refinement was being hampered by severe model bias. The high-resolution data set of the DES-hERa LBD-NR-box 2 peptide complex became available when the R_{free} of the OHT-hER α LBD model was ~31%. Both monomers in the asymmetric unit of the DES complex crystal were relocated using AMoRe and the incompletely refined OHT-hERa LBD model (with helix 12 and the loop between helices 11 and 12 removed) as the search model. The missing parts of the model were built and the rest of the model was corrected using MOLOC and two-fold averaged maps generated in DM. Initially, refinement was carried out with REFMAC using tight NCS restraints. At later stages, the model was refined without NCS restraints using the simulated annealing, minimization and B-factor refinement protocols in X-PLOR and a maximumlikelihood target. All B-factors were refined isotropically and anisotropic scaling and a bulk solvent correction were used. The R_{free} set contained a random sample of 6.5% of all data. In refinement, all data between 27 and 2.03 Å (with no σ cutoff) were used. The final model was composed of residues 305-549 of monomer A, residues 305-461 and 470-554 of monomer B, residues 687-697 of peptide A, residues 686-696 of peptide B, 164 waters, two carboxymethyl groups and a chloride ion. According to PROCHECK, 93.7% of all residues in the model were in the core regions of the Ramachandran plot and none were in the disallowed regions. Thus, the structure of the DES-hERα LBD-NR-box 2 peptide complex has been refined to a crystallographic R-factor of 19.9% (R_{free}=25.0%) using data to 2.03 Å resolution.

He 689 from the peptide interacts with three receptor residues (Asp 538, Glu 542 and Leu 539). The γ -carboxylate of Glu 542 forms hydrogen bonds to the amides of residues 689 and 690 of

the peptide. A water-mediated hydrogen bond network is formed between the imidazole ring of His 5 377, the γ -carboxylate of Glu 380, and the amide of Tyr 537. Three residues (Glu 380, Leu 536 and Tyr 537) interact with each other through van der Waals contacts and/or hydrogen bonds. Intriguingly, mutations in each these three residues dramatically increase the transcription activity of unliganded ERa LBD (Eng, et al., Mol. Cell. Biol. (1997) 17:4644-4653); Lazennec, et al., Mol. Endocrinol. (1997) 11:1375-86; White, et al., EMBO J. (1997) 16:1427-35). Atomic coordinates of 10 DES-LBD-peptide complex are attached as Appendix 2.

Table 2 Summary of Crystallographic Statistics

	-	Lig	and					
	Data Collection	DES	<u>OHT</u>					
	Space group	P2 ₁	P6 ₅ 22					
	Resolution	2.03	1.90					
	Observations	104189	269253					
	Unique	30265	23064					
	Completeness (%)	98.4	99.1					
	R _{sym} (%) ^a	7.8	7.0					
	Average Ι/σΙ	9.8	16.1					
	Refinement							
	Number of non-hydrogen atoms	4180	2070					
	R_{cryst} (%) $^b/R_{free}$ (%)	19.9/25.0	23.0/26.1					
	Bond r.m.s. deviation (Å)	0.006	0.006					
	Angle r.m.s. deviation (°)	1.05	1.05					
	Average B factor (Å ²)	34.0	40.4					
)	a $R_{sym} = \sum_i \mid I_{i^*} < I_{i^>} \mid / \sum_i I_i$ where $< I_i>$ is the average intensity							
	over symmetry equiv	alents						
	$R_{cryst} = \sum F_o - F_c / 1$	$\sum F_o $						

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C. Structure of hERα LBD-OHT complex

The OHT complex data set was then collected. Starting with one of the monomers of the preliminary low-resolution DES-hERa LBD-NR-box 2 peptide model as the search probe, molecular replacement in AMoRe was used to search for the location of LBD in this crystal form in both P6122 and P6522. A translation search in P6522 yielded the correct solution (R=53.8%, CC=38.2%). In order to reduce model bias, DMMULTI (CCP4, 1994) was then used to project averaged density from the DES complex cell into the OHT complex cell. Using MOLOC, a model of the hER α LBD was built into the resulting density. The model was refined initially in REFMAC and later with the simulated annealing, positional and B-factor refinement protocols in X-PLOR (Brunger, X-PLOR Version 3.843, New Haven, Connecticut: Yale University, 1996) using a maximum-likelihood target (Adams, et al., Proc. Natl. Acad. Sci. USA (1997) 94:5018-23). Anisotropic scaling and a bulk solvent correction were used and all B-factors were refined isotropically. Except for the Rfree set (a random sampling consisting of 8% of the data set), all data between 41 and 1.9 Å (with no σ cutoff) were included. The final model consisted of residues 306-551, the ligand and 78 waters. According to PROCHECK (CCP4, 1994), 91.6% of all residues in the model were in the core regions of the Ramachandran plot and none were in the disallowed regions. Thus, the structure of the OHT-hERa LBD complex has been refined against data of comparable resolution (1.90 Å) to a crystallographic R-factor of 23.0% (Rfree=26.2%). Atomic coordinates of OHT-hERQ LBD complex are attached as Appendix 3.

Example 17: Structural analysis of hTRß LBD:GRIP 1 NR-box 2 peptide complex

A. Structure of cocrystal complex (contents of asu)

The asymetric unit (asu) of the crystal contains two monomers of the hTR β LBD and two molecules of the GRIP1 NR-box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6), which observes the NCS relation of the two TR monomers (Figure 12). The structure of the hTR β LBD, which closely resembles that of the rTR α LBD (Wagner et al., supra), consists of twelve alpha-helices and two β -strands organized in three layers, resembling an alpha-helical sandwich. The only significant difference between the hTR β LBD and the rTR α LBD is disorder in the loop between helices H1 and H3. The GRIP1 NR-box 2 peptide forms an amphipathic α -helix of about 3 turns, preceded by 2 residues and followed by 3 residues in extended coil conformation.

The relation of the two monomers of the hTRß LBD is primarily translational, and does not resemble the homodimer structures reported for the hRXR, or the hER (Bourguet et al., <u>supra</u>;

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5 Brzozowski et al., <u>supra</u>). Furthermore, the interface between the two monomers does not involve residues necessary for formation of the physiological TR dimer. Instead, one of the cocrystal peptides appears to bridge the interaction between the two monomers. The hydrophobic face of the alpha-helix of the cocrystal peptide contacts monomer 1 of the hTRB LBD at H3, H5, and H12, while the hydrophilic face contacts monomer 2 at the hairpin turn preceding strand S3. The second cocrystal peptide also contacts monomer 2 at H3, H5, and H12, and the two cocrystal peptides observe the same NCS relation as TR LBD monomers.

The common interface between both cocrystal peptides and the hTRB LBD buries the hydrophobic residues that define the cocrystal peptide (SEQ ID NO: 1) LxxLL sequence motif, residues Ile689, Leu690, Leu693, and Leu694; against the surface of the receptor LBD (Figures 16 and 17). The presence of the second peptide in the crystal, duplicating the interactions of the hydrophobic residues, suggests those interactions are specific and drive the interaction of the peptide with the hTRB LBD, while the hydrophobic interactions provide a fortuitous crystal contact and account for the dependence of crystallization on the presence and concentration of the peptide.

B. Structure of the GRIP1 NR-box 2 peptide

The GRIP1 NR-box 2 peptide used in the crystallization is 13 amino acids long (residues 12-24 of SEQ ID NO: 6; 686-KHKILHRLLQDSS-698). For the NR-box 2 peptide in monomer 1 (peptide 1), 12 amino acids are ordered in the crystal. Residues K688 - Q694 form an amphipathic helix, with residues K686-H687 and D695-S698 on either end in extended coil conformations. For the NR-box 2 peptide in monomer 2 (peptide 2), residues K688 - Q694 again form an amphipathic helix, but the ends of the peptide are disordered. While the resolution of the current data prevents absolute assignment of hydrogen bonds, it is evident from the periodicity of the side chain density that the central residues form an alpha-helix. In the absence of TR the far UV-CD spectrum of the GRIP1 NR-box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6) appears to be random coil (data not shown). Stable helix formation may thus be induced by the interaction of the hydrophobic amino acids with the receptor LBD as it has been proposed in other protein:protein interactions, such as p53:MDM2 (Kussie et al., Science (1996) 274:948-953), VP16:TAF31 (Uesugi et al., Science (1996) 277:1310-1313), and CREB:KIX-CBP (Radhakrishnan et al., Cell (1997) 91:741-752).

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C. Structure of the hTRB LBD:GRIP1 NR-box 2 peptide interface

The hTRß LBD of the cocrystal contributes residues from three helices, H3, H5, and H12 to the interface, which pack against one another to create a hydrophobic cleft. The residues lining the cleft are 1280, T281, V283, V284, A287, and K288 from H3; Q301, I302, L305, and K306 from H5; and L454, E457, V458, and F459 from H12. A cysteine residue (C309) from H6 appears to provide a partial surface that is buried deep within the bottom of the cleft.

The GRIP1 NR-box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6) binds at the junction of H3 and H12. Leu690 of the bound peptide inserts into a shallow but defined depression at the base of the cleft, making van der Waals contact with L454 and V458 of H12, while peptide residue Ile689 packs against L454 of H12 outside the edge of the cleft; L454, then, interdigitates between the two residues. One further turn C-terminal along the alpha-helix, L693 and L694 of the bound peptide pack into complementary pockets within the hydrophobic cleft. Peptide residue L693 forms van der Waals contact with V284 of H3, while peptide residue L694, bound more deeply in the cleft, makes contact with F298 and L305 of H4 and H5. The hydrophobic interactions of the GRIP1 NR-box 2 peptide with the hTRß LBD are observed for both cocrystal peptides 1 and 2 in their respective monomers of the crystal dimer complex, suggesting that the interactions are specific to the peptide, and not induced by crystallization.

Example 18: Overall Structure of the DES-hERα-LBD-NR-box 2 Peptide Complex

The asymmetric unit of the DES-hERα LBD-NR-box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6) complex crystals contains the same noncrystallographic dimer of LBDs that has been observed in the previously determined structures of the LBD bound to both E2 and RAL (Brzozowski, et al., supra) and Tanenbaum, et al., supra). Beyond the flexible loops between helices 2 and 3 and helices 9 and 10, the two LBDs of the dimer adopt similar structures (r.m.s.d. 0.47 Å based on Cα positions). The conformation of each LBD complexed with DES closely resembles that of the LBD bound to E2 (Brzozowski, et al., supra); each monomer is a wedge shaped molecule consisting of three layers of eleven to twelve helices and a single beta hairpin. In each LBD, the hydrophobic face of helix 12 is packed against helices 3, 5/6 and 11 covering the ligand binding pocket. One NR-box 2 peptide is bound to each LBD in a hydrophobic cleft composed of residues from helices 3, 4, 5 and 12 and the turn between 3 and 4. The density for both peptides in the asymmetric unit is continuous and unambiguous. Residues 687 to 697 from peptide A and residues 686 to 696 from peptide B have been modeled; the remaining residues are disordered. Given that each peptide lies within a different environment within the crystal, it is

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5 striking that from residues Ile 689 to Gln 695 each peptide forms a two turn, amphipathic α helix. Flanking this region of common secondary structure, the peptides adopt dissimilar random coil conformations.

Example 19: Structure of the OHT-hERa LBD Complex

The binding of OHT induces a conformation of the hERα LBD that differs in both secondary and tertiary structural organization from that driven by DES binding. In the DES complex, the main chain from residues 339 to 341, 421 to 423, and 527 to 530 form parts of helices 3, 8 and 11 respectively. In contrast, these regions adopt an extended conformation in the OHT complex. In addition, the composition and orientation of helix 12 are different in the two structures. Helix 12 in the DES complex consists of residues 538 to 546 whereas helix 12 in the OHT complex consists of residues 536 to 544. Most dramatically, rather than covering the ligand binding pocket as it does in the DES complex, helix 12 in the OHT complex occupies the part of the coactivator binding groove formed by residues from helices 3, 4, and 5, and the turn connecting helices 3 and 4. This alternative conformation of helix 12 appears to be similar to that observed in the RAL complex (Brzozowski, et al., supra).

Example 20: Coactivator binding site structure and function

A. TR coactivator binding site

The above examples demonstrate that nuclear receptors, exemplified by TR, GR and ER, are recognized by specific coactivators that bind thereto through a coupling surface comprising a hydrophobic cleft and a charged hydrophobic perimeter. Identification and characterization of this coupling surface and the coactivator binding site of nuclear receptors offers a new target for the design and selection of compounds that modulate binding of coactivator to nuclear receptors.

Residues forming the coactivator binding site were found to cluster within a surprisingly small area with well-defined borders (see, e.g., Figures 5, 14, and 15). As is shown in above Examples, mutated residues nearby this area do not affect coactivator binding or transcriptional activation. Additionally, the coactivator binding assays and structural analyses demonstrated that NR-box containing proteins and peptides bind to this site. These results also showed that the GRIP1 coactivator protein binds to the site through a highly (SEQ ID NO: 1) LxxLL.

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The structural analyses showed that residues contacting a conserved leucine residue of the (SEQ ID NO: 1) LxxLL motif included V284, F293, I302, L305 and L454. Residues within 4.5Å of an atom of the bound peptide included T281, V284, K288, F293, Q301, I302, L305, K306, P453, L454 and E457. Structural analyses also revealed two other features of the site: a hydrophobic residue from helix 12 (Phe459) that contributes to local packing, and a cysteine residue contributed by helix 6 (Cys309) that provides a partial surface buried deep within the site. Mutational analyses showed that residues which block GRIP1 and SRC-1 coactivator binding when mutated are residues V284, K288, I302, K306, L454, and V458. Mutated residues likely to undergo a conformational change upon hormone binding included Leu454 and Glu457. Thus, the site identified by mutational, binding assays and crystallography corresponds to a surprisingly small cluster of residues on the surface of the LBD that define a prominent hydrophobic cleft formed by hydrophobic residues corresponding to human TR residues of C-terminal helix 3 (Ile280, Val283, Val284, and Ala287), helix 4 (Phe293), helix 5 (Ile302 and Leu305), helix 6 (Cys309), and helix 12 (Leu454, Val458 and Phe459). Collectively, the Examples indicate that residues forming the site are amino acids corresponding to human TR residues of C-terminal helix 3 (Ile280, Thr281, Val283, Val284, Ala287, and Lys288), helix 4 (Phe293), helix 5 (Gln301, Ile302, Leu305, Lvs306). helix 6 (Cys309), and helix 12 (Pro453, Leu454, Glu457, Val458 and Phe459). The coactivator binding site is highly conserved among the nuclear receptor super family (Figure 19).

The coactivator binding site of TR contains charged and hydrophobic residues at its periphery, but only hydrophobic residues at its center (see, e.g., Figures 5 and 18). The hydrophobic cleft at the center of the site may play a significant role in driving the coactivator binding reaction. The site is comprised of two parts (Figure 18), right). Residues contained in helices 3, 5 and 6 (Figure 18, yellow residues) likely form a constitutive part, since their positions are identical in all nuclear receptor structures reported, including the liganded, activated states of the TR, RAR, and ER, the unliganded RXR, and the inhibitor-liganded ER. By contrast, the residues of helix 12 (Figure 18, red residues) are differently positioned in the active and inactive states reported. Thus the coactivator binding site for the nuclear receptors is likely to be formed in response to an active hormone by positioning helix 12 against a scaffold formed by helices 3-6. Because the coactivator binding site is so small, it is easy to understand how even slight changes in the position of helix 12, which may, for example, be induced by an antagonist ligand, could impair coactivator binding, and thus receptor activation.

B. ER coactivator binding site

Binding of the NR-box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6) to the ER α LBD buries 1000 Å² of predominantly hydrophobic surface area from both molecules. The NR-box 2 peptide binding site is a shallow groove composed of residues Leu 354, Val 355, Ile 358, Ala 361 and Lys 362 from helix 3; Phe 367 and Val 368 from helix 4; Leu 372 from the turn between helices 3 and 4; Gln 375, Val 376, Leu 379 and Glu 380 from helix 5; and Asp 538, Leu 539, Glu 542 and Met 543 from helix 12. The floor and sides of this groove are completely nonpolar, but the ends of this groove are charged. Therefore, structural characterization of the binding site of the NR-box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6) to the ER α LBD, which is the same NR-box 2 peptide utilized to crystallize the T₃-TR LBD, supports the findings for TR that residues forming the coactivator binding site of nuclear receptors is composed of a well defined hydrophobic cleft and a charged hydrophobic perimeter. These residues are highly conserved among the nuclear receptor super family (Figure 19). Structural characterization of the coactivator peptide-bound ER LBD also supports the concept of exploiting the slight differences among the coactivator binding sites of nuclear receptors in designing and identifying compounds that target specific nuclear receptors.

The ERα LBD interacts primarily with the hydrophobic face of the NR-box 2 peptide 686-KHKILHRLLQDSS-698 (residues 12-24 of SEQ ID NO: 6) α helix formed by the side chains of Ile 689 and the three (SEQ ID NO: 1) LxxLL motif leucines (Leu 690, Leu 693 and Leu 694). The side chain of Leu 690 is deeply embedded within the groove and forms van der Waals contacts with the side chains of Ile 358, Val 376, Leu 379, Glu 380 and Met 543. The side chain of Leu 694 is similarly isolated within the groove and makes van der Waals contacts with the side chains of Ile 358, Lys 362, Leu 372, Gln 375, Val 376 and Leu 379. In contrast, the side chains of both Ile 689 and the second NR box leucine, Leu 693, rest against the rim of the groove. The side chain of Ile 689 lies in a shallow depression formed by the side chains of Asp 538, Leu 539 and Glu 542. The side chain of Leu 693 makes nonpolar contacts with the side chains of Ile 358 and Leu 539.

The charged and polar side chains which form the hydrophilic face of the peptide helix project away from the ER α receptor and either interact predominantly with solvent or form symmetry contacts. None of the side chains of the polar and charged residues outside the helical region of either peptide in the asymmetric unit, with the exception of Lys 688 of peptide B, is involved in hydrogen bonds or salt bridges with its associated ER α LBD monomer. The ϵ -amino group of Lys 688 of peptide B hydrogen bonds to the side chain carboxylate of Glu 380 of monomer B. This interaction is presumably a crystal artifact; the main chain atoms of the N-

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5 terminal three residues of peptide B are displaced from monomer B and interact extensively with a symmetry-related ERα LBD.

In addition to interacting with the hydrophobic face of the peptide helix, the ER α LBD stabilizes the main chain conformation of the NR box peptide by forming capping interactions with both ends of the peptide helix. Glu 542 and Lys 362 are positioned at opposite ends of the peptide binding site. The side chains of Glu 542 and Lys 362 form van der Waals contacts with main chain and side chain atoms at the N- and C-terminal turns of the peptide helix respectively. These interactions position the stabilizing charges of the γ -carboxylate of Glu 542 and ϵ -amino group of Lys 362 near the ends of the NR box peptide helix. The side chain carboxylate of Glu 542 hydrogen bonds to the amides of the residues of N-terminal turn of the peptide helix (residues 688 and 689 of peptide A; residues 689 and 690 of peptide B). Similarly, the ϵ -amino group of Lys 362 hydrogen bonds to the carbonyls of the residues of the C-terminal turn of the peptide helix (residue 693 of peptide A; residues 693 and 694 of peptide B).

Except for the orientation of helix 12, the structure of the peptide binding groove of the ER α LBD is almost identical in the DES and OHT complexes. The region of this groove outside of helix 12 is referred to herein as the "static region" of the NR box binding site. Helix 12 in the OHT complex and the NR box peptide helix in the DES complex interact with the static region of the coactivator recognition groove in strikingly similar ways.

Helix 12 mimics the hydrophobic interactions of the NR box peptide with the static region of the groove with a stretch of residues (residues 540 to 544) that resembles an NR box ((residues 6-10 of SEQ ID NO: 43) LLEML instead of (SEQ ID NO: 1) LxxLL). The side chains of Leu 540 and Met 543 lie in approximately the same locations as those of the first and second motif leucines (Leu 690 and Leu 693) in the peptide complex. Leu 540 is inserted into the groove and makes van der Waals contacts with Leu 354, Val 376 and Glu 380. Met 543 lies along the edge of the groove and forms van der Waals contacts with the side chains of Leu 354, Val 355 and Ile 358. The side chain position of Leu 544 almost exactly overlaps that of the third NR box leucine, Leu 694. Deep within the groove, the Leu 544 side chain makes van der Waals contacts with the side chains of Ile 358, Lys 362, Leu 372, Gln 375, Val 376 and Leu 379.

Helix 12 in the OHT complex is also stabilized by N- and C-terminal capping interactions. Lys 362 interacts with the C-terminal turn of helix 12 much as it does with the equivalent turn of the peptide helix. The Lys 362 side chain packs against the C-terminal turn of the helix 12 with its \(\varepsilon\)-amino group hydrogen bonding to the carbonyls of residues 543 and 544. Given that the capping

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5 interaction at the N-terminal turn coactivator helix is formed by a helix 12 residue (Glu 542), the N-terminal turn of helix 12 in the antagonist complex is forced to interact with another residue, Glu 380. The Glu 380 γ-carboxylate forms van der Waals contacts with Tyr 537 and interacts with the amide of Tyr 537 through a series of water-mediated hydrogen bonds.

In addition to forming these "NR box-like" interactions, helix 12 also forms van der Waals contacts with areas of the ER α LBD outside of the coactivator recognition groove. The side chain of Leu 536 forms van der Waals contacts with Glu 380 and Trp 383 and that of Tyr 537 forms van der Waals contacts with His 373, Val 376 and Glu 380. As a result of these contacts, helix 12 in the OHT complex buries more solvent accessible surface area (~1200 Å 2) than the NR box peptide in the DES-ER α LBD-peptide complex.

Identification and characterization of the coactivator binding site for TR, and extension of this information to other nuclear receptors shows that this site is common for all nuclear receptors identified to date. Additionally, sequence and structural comparison, coupled with the Examples showing differential specificity for coactivator binding to TR, GR and ER, reveal that minor differences between the receptors, such as found in helix 12, are likely to influence specificity of a coactivator for different types of nuclear receptors. Thus, the Examples presented herein demonstrate that information derived from the structure and function of the TR coactivator binding site can be applied in design and selection of compounds that modulate binding of coactivator proteins to nuclear receptors for all members of the nuclear receptor super family.

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All publications and patent applications mentioned in this specification are herein 35 incorporated by reference to the same extent as if each individual publication or patent application was specifically and individually indicated to be incorporated by reference.

5 The invention now being fully described, it will be apparent to one of ordinary skill in the art that many changes and modifications can be made thereto without departing from the spirit or scope of the appended claims.

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WHAT IS CLAIMED IS:

 A method of identifying a compound that modulates coactivator binding to a nuclear receptor, said method comprising:

modeling test compounds that fit spacially into a nuclear receptor coactivator binding site of interest using an atomic structural model of a nuclear receptor coactivator binding site or portion thereof.

screening said test compounds in an assay characterized by binding of a test compound to a nuclear receptor coactivator binding site, and

identifying a test compound that modulates coactivator binding to said nuclear receptor.

- The method of claim 1, wherein said atomic structural model comprises atomic coordinates of amino acid residues corresponding to residues of human thyroid receptor selected from the group consisting of Val284, Phe293, Ile302, Leu305, and Leu454.
- The method of claim 1, wherein said atomic structural model comprises atomic coordinates of amino acid residues corresponding to residues of human thyroid receptor selected from the group consisting of Val284, Lys288, Ile302, Lys306, Leu454 and Glu457.
- 4. The method of claim 1, wherein said atomic structural model comprises atomic coordinates of amino acid residues corresponding to residues of human thyroid receptor helix 3 residues Ile280, Thr281, Val283, Val284, Ala287, and Lys288, helix 4 residue Phe293, helix 5 residues Gln301, Ile302, Leu305, Lys306, helix 6 residue Cys309, and helix 12 residues Pro453, Leu454, Glu457, Val458 and Phe459.
- 5. The method of claim 1, wherein said nuclear receptor coactivator binding site comprises amino acid residues corresponding to residues of human thyroid receptor selected from the group consisting of helix 3 residues Ile280, Thr281, Val283, Val284, Ala287, and Lys288, helix 4 residue Phe293, helix 5 residues Gln301, Ile302, Leu305, Lys306, helix 6 residue Cys309, and helix 12 residues Pro453, Leu454, Glu457, Val458 and Phe459.
- The method of claim 5, wherein said amino acid residues corresponding to residues of human thyroid receptor comprise Val284, Phe293, Ile302, Leu305, and Leu454.

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- The method of claim 5, wherein said amino acid residues corresponding to residues of human thyroid receptor comprise Val284, Lys288, Ile302, Lys306, Leu454 and Glu457.
- 8. The method of claim 1, wherein said nuclear receptor coactivator binding site comprises amino acid residues corresponding to residues of human thyroid receptor of helix 3 residues Ile280, Thr281, Val283, Val284, Ala287, and Lys288, helix 4 residue Phe293, helix 5 residues Gln301, Ile302, Leu305, Lys306, helix 6 residue Cys309, and helix 12 residues Pro453, Leu454, Glu457, Val458 and Phe459.
 - The method of any one of claims 5 through 8, wherein said nuclear receptor is selected from the group consisting of TR, RAR, RXR, PPAR, VDR, ER, GR, PR, MR, and AR.
 - 10. The method of claim 1, wherein said screening is in vitro.
 - 11. The method of claim 10, wherein said screening is high throughput screening.
 - 12. The method of claim 1, wherein said assay is a biological assay.
 - 13. The method of claim 1, wherein said test compound is from a library of compounds.
 - The method of claim 1, wherein said test compound is an agonist or antagonist of coactivator binding.
- 15. The method of claim 14, wherein said test compound is a small organic molecule, a 30 peptide, or peptidomimetic.
 - The method of claim 15, wherein said compound is a peptide comprising a NR-box amino acid sequence, or derivative thereof.
- 35 17. A method for identifying an agonist or antagonist of coactivator binding to a nuclear receptor, said method comprising the steps of:

providing the atomic coordinates of a nuclear receptor coactivator binding site or portion thereof to a computerized modeling system;

modeling compounds which fit spacially into the nuclear receptor coactivator binding site; and

identifying in an assay for nuclear receptor activity a compound that increases or decreases the activity of said nuclear receptor by binding the coactivator binding site of said nuclear receptor, whereby an agonist or antagonist of coactivator binding is identified.

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- 18. A machine-readable data storage medium, comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of a molecular complex of a compound bound to a nuclear receptor coactivator binding site comprising structure coordinates of amino acids corresponding to human thyroid receptor amino acids selected from the group consisting of helix 3 residues Ile280, Thr281, Val283, Val284, Ala287, and Lys288, helix 4 residue Phe293, helix 5 residues Gln301, Ile302, Leu305, Lys306, helix 6 residue Cys309, and helix 12 residues Pro453, Leu454, Glu457, Val458 and Phe459, or a homologue of said molecular complex, wherein said homologue comprises a coactivator binding site that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.
- The machine readable storage medium of claim 18, wherein said nuclear receptor is a thyroid receptor.
- The machine readable storage medium of claim 19, wherein said thyroid receptor is human.
 - 21. The machine readable storage medium of claim 20, wherein said molecule is peptide.
- The machine readable storage medium of claim 21, wherein said peptide comprises a NR-box amino acid sequence, or derivative thereof.
 - 23. The machine-readable data storage medium according to claim 18, wherein said molecular complex is defined by the set of structure coordinates depicted in Appendix 1, or a homologue of said molecular complex, said homologue having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.
 - 24. A machine-readable data storage medium comprising a data storage material encoded with a first set of machine readable data which, when combined with a second set of

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- 5 machine readable data, using a machine programmed with instructions for using said first set of data and said second set of data, can determine at least a portion of the structure coordinates corresponding to the second set of machine readable data, wherein: said first set of data comprises a Fourier transform of at least a portion of the structural coordinates selected from the group consisting of coordinates depicted in Appendix 1; and said second set of data comprises an X-ray
 10 diffraction pattern of a molecule or molecular complex.
 - A cocrystal of a nuclear receptor comprising a molecule bound to the coactivator binding site of said nuclear receptor.
 - 26. The cocrystal of claim 25, wherein said nuclear receptor is a thyroid receptor.
 - 27. The cocrystal of claim 26, wherein said thyroid receptor is human.
 - 28. The cocrystal of claim 27, wherein said molecule is peptide.
 - The cocrystal of claim 28, wherein said peptide comprises a NR-box amino acid sequence or derivative thereof.
 - 30. A compound identified according to the method of claim 1.

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MOTA

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Atomic Coordinates for Human TR-B Complexed With T3, and a GRIP1 NR-box 2 Peptide

REMARK full length numbering REMARK all residue names correct 10 REMARK peptide sequence REMARK two molecules of TRB - CHAIN A and CHAIN B REMARK two molecules of T3 - CHAIN J and CHAIN K REMARK two molecules of GRIP-1 peptide - CHAIN X and CHAIN Y REMARK chain X lies between A and B 15 REMARK chain Y interacts with B only REMARK residues differing between A and B include: REMARK A 217 Glu, A 252 Gln, A 263 Lys (missing side chains) REMARK B 237 Ser, B239 His, B 394 Lys (missing side chains) REMARK additionally Gly 261, Gly 262 are not visible in chain A 20 REMARK residues differing between X and Y include: REMARK A 692 Arg REMARK additionally, residues Lys 688, Lys 689; Ser 697, Ser 698 REMARK are not visible in chain Y 23.912 35.239 1.00 45.76 25 LYS A 211 52.546 MOTA 1 N 24.345 36.586 1.00 43.42 2 CA LYS A 211 52.944 MOTA LYS A 211 52.035 23.665 37.836 1.00 35.68 MOTA 3 C 22.556 37.763 1.00 33.58 ATOM 0 LYS A 211 51.511 1.00 46.72 36.779 LYS A 211 52.610 25.825 ATOM 5 CB 7 24.182 39.199 1.00 35.64 30 PRO A 212 51.678 ATOM 6 N 52.082 25.474 39.842 1.00 38.60 6 7 CD PRO A 212 ATOM 8 CA PRO A 212 50.809 23.379 40.166 1.00 38.35 MOTA 41.440 1.00 38.95 CB PRO A 212 50.670 24.194 ATOM 9 41.255 1.00 42.00 CG PRO A 212 51.455 25.469 ATOM 10 49.433 23.097 39.594 1.00 38.78 PRO A 212 35 MOTA 11 С PRO A 212 48.920 23.949 38.802 1.00 34.64 MOTA 12 0 7 48.901 21.948 40.014 1.00 40.31 MOTA 13 N GLU A 213 14 CA GLU A 213 39.529 1.00 43.87 47.609 21.419 ATOM 47.943 20.307 38.520 1.00 45.16 15 CB GLU A 213 ATOM 16 CG GLU A 213 49.125 20.708 37.601 1.00 47.60 6 40 ATOM 1.00 50.68 6 17 CD GLU A 213 49.284 19.828 36.353 MOTA OE1 GLU A 213 49.355 18.547 36.474 1.00 59.18 MOTA 18 8 OE2 GLU A 213 49.356 20.368 35.180 1.00 49.06 19 ATOM 46.711 20.988 1.00 45.96 6 GLU A 213 40.747 ATOM 20 С GLU A 213 47.111 21.136 41.910 1.00 43.13 45 ATOM 21 0 7 40.515 1.00 46.52 ATOM 22 PRO A 214 45.463 20.460 39.148 1.00 46.44 CD PRO A 214 44.985 20.184 ATOM 23 41.596 1.00 47.52 6 PRO A 214 44.447 20.124 ATOM 24 CA 43.249 19.629 40.816 1.00 45.40 6 25 PRO A 214 ATOM CB 26 CG PRO A 214 43.588 19.674 39.327 1.00 49.89 50 MOTA 1.00 45.70 42.625 ATOM 27 C PRO A 214 44.787 19.082 42.535 1.00 44.49 8 45.816 18.466 ATOM 28 O PRO A 214 7 43.915 18.876 43.606 1.00 45.24 29 THR A 215 ATOM N 17.890 44.686 1.00 49.36 6 30 CA THR A 215 44.161 MOTA 1.00 44.86 31 CB THR A 215 44.163 18.586 46.093 55 ATOM 1.00 52.26 42.878 18.447 46.728 ATOM 32 OG1 THR A 215 20.031 45.974 1.00 39.43 CG2 THR A 215 44.514 ATOM 33

16.995

THR A 215

44.667

1.00 52.51

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		ATOM	92	CG2	ILE	Α	222	35.970	21.182	37.893	1.00	28.86	6
		ATOM	93	CG1	ILE	Α	222	37.532	21.922	39.707	1.00	33.33	6
	10	ATOM	94	CD1	ILE			38.804	21.586	39.004	1.00	34.85	6
	10	ATOM	95	C	ILE			34.067	20.365	39.735	1.00	34.26	6
		ATOM	96	0	ILE			33.033	20.873	39.319		31.90	8
			97	N	LYS			34.301	19.058	39.750		39.49	7
		ATOM						33.316	18.100	39.276		44.43	6
		ATOM	98	CA	LYS				16.713	39.852		50.81	6
	15	ATOM	99	CB	LYS			33.603				62.51	6
		ATOM	100	CG	LYS			32.741	15.631	39.227			6
		MOTA	101	CD	LYS			32.859	14.291	39.943		72.22	
		MOTA	102	CE	LYS			31.798	13.318	39.430		74.55	6
		ATOM	103	NZ	LYS			31.900	11.985	40.106		75.78	7
	20	ATOM	104	С	LYS	Α	223	31.913	18.565	39.681		42.81	6
		ATOM	105	0	LYS	Α	223	30.936	18.323	38.984		40.36	8
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		ATOM	107	CA	THR	Α	224	30.602	19.792	41.378	1.00	39.93	6
75		ATOM	108	CB	THR	Α	224	30.805	20.206	42.851	1.00	40.57	6
0	25	ATOM	109	OG1	THR	Α	224	31.330	19.113	43.616	1.00	39.27	8
17.1		ATOM	110	CG2	THR			29.500	20.684	43.461	1.00	38.11	6
ii)		ATOM	111	C	THR			30.167	21.011	40.533	1.00	39.96	6
1.6		ATOM	112	Ö	THR			29.313	20.899	39.655	1.00	36.67	8
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21			116		VAL			31.512	25.636	39.491		36.77	6
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E.	35	MOTA	119	0	VAL			30.783	22.316	38.018		34.02	7
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	40	ATOM	124		THR			31.108	20.346	34.783		20.99	6
		MOTA	125	С			226	29.100	21.361	36.510		36.41	6
		MOTA	126	0			226	28.255	21.877	35.785		39.64	8
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	45	ATOM	129	CB	ALA	А	227	27.526	18.600	38.381		38.06	6
		ATOM	130	С	ALA	Α	227	26.507	20.604	37.318		37.69	6
		ATOM	131	0	ALA	Α	227	25.444	20.489	36.718	1.00	40.94	8
		ATOM	132	N	ALA	Α	228	26.811	21.630	38.107	1.00	32.86	7
		ATOM	133	CA	ALA	Α	228	25.903	22.734	38.356	1.00	32.48	6
	50	ATOM	134	CB	ALA	Α	228	26.448	23.587	39.486	1.00	28.25	6
	20	ATOM	135	c			228	25.732	23.570	37.101	1.00	36.12	6
		ATOM	136	ō			228	24.673	23.560	36.473	1.00	37.86	8
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			138	CA			229	26.762	25.158	35.585		32.97	6
	55	ATOM	130	CB			229	28.155	25.691	35.266		33.69	6
	33	ATOM			HIS		229	28.250	26.333	33.929		28.39	6
		ATOM	140	CG				29.025	26.081	32.838		28.83	6
		ATOM	141		HIS			27.386	27.368	33.542		30.47	7
		MOTA	142	NDI	HIS	А	229	21.300	21.300	33.342	1.00	30.47	

	5	ATOM	143	CE1	HIS	Α	229	27.654	27.692	32.280	1.00	26.95	6
		ATOM	144	NE2	HIS	Α	229	28.635	26.934	31.840	1.00	31.27	7
		ATOM	145	С	HIS	Α	229	26.225	24.541	34.312	1.00	38.40	6
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		ATOM	152	С	VAL	Α	230	24.603	22.239	32.900	1.00	44.28	6
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		ATOM	154	N	ALA			24.072	21.862	34.059	1.00	45.59	7
		ATOM	155	CA	ALA			22.669	21.500	34.175	1.00	47.84	6
		ATOM	156	СВ	ALA			22.482	20.582	35.374	1.00	45.08	6
		ATOM	157	C	ALA			21.792	22.734	34.314	1.00	48.04	6
	20	ATOM	158	0	ALA			20.565	22.647	34.324	1.00	49.95	8
		ATOM	159	N	THR			22.436	23.894	34.384	1.00	47.26	7
		ATOM	160	CA	THR			21.722	25.161	34.528	1.00	43.64	6
		ATOM	161	CB	THR			22.112	25.832	35.850	1.00	41.93	6
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111		ATOM	164	С	THR			22.055	26.114	33.387	1.00	43.97	6
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34.2		ATOM	167	CA	ASN			23.134	26.468	31.231	1.00	58.62	6
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St.	50	ATOM	169	CG	ASN			25.141	27.355	29.927	1.00	68.35	6
41		ATOM	170		ASN			24.822	28.544	30.096	1.00	65.50	8
Francisco (ATOM	171	ND2	ASN	Α	233	25.951	26.951	28.959	1.00	74.29	7
1,0		ATOM	172	С	ASN	Α	233	22.241	26.035	30.073	1.00	65.06	6
1,4	35	ATOM	173	0	ASN	Α	233	22.312	24.900	29.604	1.00	69.47	8
10		ATOM	174	N	ALA	Α	234	21.381	26.954	29.646	1.00	68.80	7
ñ		ATOM	175	CA	ALA	Α	234	20.423	26.708	28.564	1.00	70.98	6
182		MOTA	176	CB	ALA	Α	234	19.748	28.015	28.186	1.00	71.43	6
		ATOM	177	C	ALA	Α	234	20.988	26.062	27.308	1.00	73.83	6
	40	MOTA	178	0	ALA	Α	234	22.041	26.419	26.822	1.00	74.33	8
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		ATOM	180	CA	GLN	Α	235	20.562	24.363	25.629		76.32	6
		ATOM	181	CB	GLN	Α	235	20.328	25.239	24.391		76.98	6
		ATOM	182	CG	GLN	Α	235	18.887	25.292	23.908		77.07	6
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		ATOM	184	OE1	GLN	Α	235	17.668	24.448	25.768		82.01	8
		ATOM	185	NE2	GLN	Α	235	17.313	26.596	25.149		78.80	7
		ATOM	186	С	GLN	Α	235	21.960	23.840	25.573		77.15	6
		ATOM	187	0	GLN	Α	235	22.386	23.458	24.508		76.06	8
	50	ATOM	188	N	GLY	Α	236	22.676	23.766	26.687		77.46	7
		ATOM	189	CA	GLY	Α	236	24.053	23.245	26.627		78.37	6
		ATOM	190	С	GLY	Α	236	24.923	23.491	25.390		79.43	6
		ATOM	191	0	GLY	Α	236	24.917	24.565	24.844		79.47	8
		ATOM	192	N	SER	Α	237	25.739	22.526	24.991		77.98	7
	55	ATOM	193	CA	SER	Α	237	26.566	22.760	23.801		76.49	6
		ATOM	194	CB	SER	Α	237	27.981	22.206	24.015		76.46	6
		ATOM	195	OG	SER	Α	237	28.821	23.145	24.689		40.00	8
		ATOM	196	C	SER	Α	237	25.938	22.127	22.542	1.00	75.35	6

	_					_		0.5.505	04 410	01 707	1 00	75.47	8
	5	ATOM	197	0	SER			26.605	21.418	21.797			
		ATOM	198	N	HIS			24.648	22.410	22.353		75.56	7
		ATOM	199	CA	HIS	Α	238	23.842	21.981	21.236		75.46	6
		ATOM	200	CB	HIS	Α	238	22.990	20.732	21.661		75.85	6
		ATOM	201	CG	HIS	Α	238	22.408	19.933	20.542	1.00	40.00	6
	10	ATOM	202	CD2	HIS	А	238	22.790	18.757	19.957	1.00	40.00	6
		ATOM	203		HIS			21.223	20.303	19.875	1.00	40.00	7
					HIS			20.951	19.365	18.953		40.00	6
		ATOM	204					21.874	18.444	18.994		40.00	7
		ATOM	205		HIS							74.10	6
		ATOM	206	С	HIS			22.971	23.284	20.964			
	15	ATOM	207	0	HIS			21.863	23.137	20.441		75.34	8
		ATOM	208	И	TRP	А	239	23.487	24.510	21.368		73.39	7
		ATOM	209	CA	TRP	Α	239	22.872	25.894	21.195		74.02	6
		ATOM	210	CB	TRP	Α	239	23.563	27.026	22.005	1.00	81.77	6
		ATOM	211	CG	TRP	Α	239	25.022	27.366	21.688	1.00	89.67	6
	20	ATOM	212	CD2	TRP	Α	239	25.532	28.662	21.240	1.00	93.19	6
		ATOM	213	CE2	TRP			26.961	28.522	21.136	1.00	95.46	6
		ATOM	214	CE3	TRP			24.936	29.911	20.969	1.00	95.35	6
		ATOM	215		TRP			26.102	26.548	21.781	1.00	94.16	6
1775		ATOM	216	NE1				27.268	27.241	21.475		97.48	7
10	25		217	CZ2	TRP			27.798	29.598	20.764		96.23	6
111	23	ATOM			TRP			25.763	30.967	20.569		96.75	6
10		ATOM	218							20.482		97.32	6
1.62 1.63		ATOM	219		TRP			27.171	30.825				
		ATOM	220	С	TRP			22.799	26.407	19.774		70.77	6
N		ATOM	221	0	TRP			21.706	26.562	19.263		71.70	8
Soli	30	ATOM	222	N	LYS			23.946	26.701	19.157		67.10	7
144		MOTA	223	CA	LYS	Α	240	23.978	27.180	17.783		65.63	6
93 Jane		ATOM	224	CB	LYS	Α	240	25.314	26.780	17.153		66.65	6
		ATOM	225	CG	LYS	Α	240	26.529	27.342	17.872		69.83	6
		ATOM	226	CD	LYS	Α	240	27.805	27.037	17.108	1.00	71.49	6
1.1	35	ATOM	227	CE	LYS	Α	240	28.980	27.720	17.776	1.00	71.31	6
		MOTA	228	NZ	LYS	Α	240	30.238	27.438	17.034	1.00	72.23	7
10		ATOM	229	С	LYS			22.808	26.699	16.895	1.00	66.19	6
ר		ATOM	230	o	LYS			22.550	27.298	15.851	1.00	65.20	8
		ATOM	231	N	ASN			22.113	25.640	17.325		66.69	7
	40	ATOM	232	CA	ASN			20.976	25.078	16.599		67.53	6
	+0		233	CB	ASN			21.122	23.562	16.550		67.98	6
		ATOM		CG			241	22.304	23.121	15.693		70.19	6
		MOTA	234					22.404	23.506	14.503		71.37	8
		ATOM	235		ASN					16.271		71.48	7
		MOTA	236		ASN			23.176	22.310				6
	45	ATOM	237	С			241	19.570	25.421	17.152		66.62	
		ATOM	238	0			241	18.581	24.822	16.731		64.76	8
		ATOM	239	N	LYS	Α	242	19.475	26.380	18.069		66.86	7
		ATOM	240	CA	LYS	Α	242	18.191	26.786	18.642		67.46	6
		ATOM	241	CB	LYS	Α	242	18.164	26.396	20.119		67.93	6
	50	ATOM	242	CG	LYS	Α	242	18.250	24.896	20.337		71.52	6
		ATOM	243	CD	LYS	Α	242	17.004	24.149	19.821	1.00	74.32	6
		ATOM	244	CE			242	15.755	24.491	20.643	1.00	74.41	6
		ATOM	245	NZ			242	15.927	24.161	22.109	1.00	74.44	7
		ATOM	246	C			242	18.143	28.291	18.483		66.28	6
	55	ATOM	247	0			242	17.102	28.923	18.592		67.61	8
	23	ATOM	248	N			243	19.334	28.813	18.204		64.19	7
			249	CA			243	19.617	30.219	17.975		62.43	6
		ATOM		CB			243	21.070	30.274	17.463		60.12	6
		MOTA	250	CD	ANG	А	243	21.070	50.274	27.200	1.00	30.12	-

									22 626	17 205	1 00	40.00	6
	5	ATOM	251	CG	ARG			21.665	31.636	17.305			
		ATOM	252	CD	ARG	Α	243	23.213	31.599	17.267		40.00	6
		ATOM	253	NE	ARG	Α	243	23.826	31.217	15.996	1.00	40.00	7
		ATOM	254	CZ	ARG	Α	243	25.113	31.439	15.714	1.00	40.00	6
		ATOM	255	NH1	ARG	Α	243	25.905	32.041	16.616	1.00	40.00	7
	10	ATOM	256		ARG			25.592	31.097	14.520	1.00	40.00	7
	10	ATOM	257	C	ARG			18.639	30.789	16.950	1.00	62.97	6
			258	0	ARG			18.662	30.390	15.784		63.96	8
		ATOM							31.692	17.393		62.41	7
		ATOM	259	N	LYS			17.771				61.57	6
		ATOM	260	CA	LYS			16.790	32.309	16.498			6
	15	ATOM	261	CB	LYS			15.368	31.974	16.962		63.68	
		ATOM	262	CG	LYS			15.102	30.471	17.104		71.29	6
		ATOM	263	CD	LYS	Α	244	13.641	30.167	17.468		73.83	6
		ATOM	264	CE	LYS	Α	244	13.182	30.908	18.737		74.71	6
		ATOM	265	NZ	LYS	Α	244	13.951	30.536	19.970		73.32	7
	20	ATOM	266	С	LYS	Α	244	17.009	33.806	16.501		59.30	6
		ATOM	267	0	LYS	Α	244	16.562	34.514	17.399	1.00	56.34	8
		ATOM	268	N	PHE	Α	245	17.705	34.264	15.468	1.00	57.06	7
		ATOM	269	CA	PHE	Α	245	18.045	35.692	15.333	1.00	59.01	6
100		ATOM	270	CB	PHE			18.825	35.947	14.049	1.00	59.62	6
10	25	ATOM	271	CG	PHE			19.908	34.979	13.834	1.00	66.60	6
113	23	ATOM	272		PHE			19.618	33.714	13.399	1.00	67.17	6
10			273		PHE			21.198	35.309	14.139		69.25	6
lat.		ATOM			PHE			20.614	32.794	13.255		69.92	6
14		ATOM	274					22.189		13.994		70.50	6
įut.	20	MOTA	275	CE2	PHE					13.552		70.89	6
14	30	ATOM	276	CZ	PHE			21.897		15.340		60.68	6
16 12		ATOM	277	С	PHE			16.856				62.37	8
125		ATOM	278	0	PHE			15.946		14.528			
1,0		ATOM	279	N	LEU			16.919		16.272		60.10	7
149		ATOM	280	CA			246	15.884		16.437		59.44	6
	35	ATOM	281	CB	LEU			16.227		17.585		57.43	6
10		ATOM	282	CG	LEU	Α	246	15.100		18.086		54.41	6
٠. (D		ATOM	283	CD1	LEU	Α	246	14.010	39.474	18.640		52.43	6
100		ATOM	284	CD2	LEU	Α	246	15.575		19.151		51.69	6
		ATOM	285	С	LEU	Α	246	15.717	39.330	15.135	1.00	62.05	6
	40	ATOM	286	0	LEU	Α	246	16.706	39.609	14.430		59.85	8
		ATOM	287	N	PRO	Α	247	14.473	39.668	14.784	1.00	63.33	7
		ATOM	288	CD	PRO	Α	247	13.263	39.314	15.534	1.00	64.44	6
		ATOM	289	CA			247	14.198		13.558	1.00	63.56	6
		ATOM	290	CB			247	12.687	40.671	13.600	1.00	64.42	6
	45	ATOM	291	CG			247	12.161		14.729	1.00	64.90	6
	43	ATOM	292	C			247	14.996		13.496	1.00	61.94	6
			293	0			247	15.159		14.486		61.60	8
		ATOM					248	15.506		12.299		61.33	7
		ATOM	294	N						11.976		63.50	6
		MOTA	295	CA			248	16.280		10.437		66.94	6
	50	ATOM	296	CB			248	16.481		9.966		68.70	6
		ATOM	297	CG			248	17.012					6
		ATOM	298	CD			248	16.981		8.471		40.00	
		ATOM	299		GLU			16.432		7.644		40.00	8
		ATOM	300	OE2			248	17.509		8.086		40.00	8
	55	ATOM	301	С			248	15.624		12.458		64.19	6
		ATOM	302	0	GLU	Α	248	16.298		12.918		65.56	8
		MOTA	303	N	ASP	Α	249	14.300	44.545	12.323		64.36	7
		ATOM	304	CA	ASP	Α	249	13.493	45.703	12.673	1.00	63.33	6

	5	ATOM	73	CG	PHE A	A 2	272	15.953	42.413	25.282	1.00	33.39	6
		ATOM	74	CD1	PHE A	A 2	272	16.619	43.615	25.093	1.00	33.14	6
		ATOM	75	CD2	PHE 2	A 2	272	16.138	41.394	24.346	1.00	38.28	6
		ATOM	76	CE1	PHE 2	A 2	272	17.454	43.807	23.988	1.00	38.26	6
		ATOM	77	CE2	PHE 2			16.973	41.585	23.244	1.00	43.28	6
	10	ATOM	78	CZ	PHE 2			17.634	42.786	23.068	1.00	39.74	6
		ATOM	79	С	PHE 2			13.650	40.528	27.764	1.00	40.75	6
		ATOM	80	0	PHE 2			14.081	39.476	28.227	1.00	35.51	8
		ATOM	81	N	THR 2			12.756	41.266	28.428	1.00	41.64	7
		ATOM	82	CA	THR .			12.290	40.854	29.757	1.00	45.97	6
	15	ATOM	83	CB	THR .			11.651	42.025	30.506		51.52	6
	13	ATOM	84	OG1	THR .			10.442	42.422	29.859	1.00	45.74	8
		ATOM	85	CG2	THR			12.601	43.211	30.565	1.00	49.73	6
		ATOM	86	C	THR .			11.267	39.731	29.664	1.00	46.23	6
		ATOM	87	0	THR .			10.854	39.183	30.680		41.21	8
	20	ATOM	88	N	LYS .			10.849	39.412	28.440		46.21	7
	20	ATOM	89	CA	LYS			9.871	38.362	28.211		54.53	6
		ATOM	90	CB	LYS .			9.414	38.405	26.773		54.36	6
		ATOM	91	С	LYS			10.498	37.015	28.515		56.88	6
g144g		ATOM	92	0	LYS			9.789	36.044	28.759		57.98	8
10	25	ATOM	93	N	ILE			11.836	36.973	28.491		56.48	7
TU	23	ATOM	94	CA	ILE			12.609	35.746	28.767		52.64	6
10		ATOM	95	CB	ILE			13.444	35.346	27.543		49.15	6
Turks Sweet		ATOM	96	CG2	ILE			12.568	34.829	26.429		47.42	6
4		ATOM	97		ILE			14.238	36.532	27.026		45.31	6
Irale	30		98		ILE			15.001	36.242	25.771		37.22	6
1	30	ATOM	99	C	ILE			13.541	35.870	29.982		51.78	6
82		ATOM ATOM	100	0	ILE			14.014	34.873	30.503		49.80	8
£250			101	N	ILE			13.790	37.107	30.415		51.76	7
1,1		ATOM	102	CA	ILE			14.681	37.389	31.537		52.58	6
(J	35	ATOM ATOM	103	CB	ILE			14.691	38.877	31.844		55.04	6
120	33	ATOM	103	CG2	ILE			13.311	39.340	32.261		53.28	6
10			105	CG1	ILE			15.675	39.206	32.976		57.31	6
923		ATOM	106	CD1				17.096	38.942	32.655		60.32	6
		ATOM ATOM	107	CDI	ILE			14.323	36.644	32.828		50.70	6
	40		108	0	ILE			15.177	36.458	33.691		55.55	8
	40	ATOM ATOM	100	N	THR			13.072	36.209	32.963		47.33	7
		ATOM	110	CA	THR			12.631	35.523	34.158		42.59	6
			111	CB	THR			11.098	35.456	34.217		44.97	6
		ATOM ATOM	112		THR			10.545	36.777	34.102		46.38	8
	45		113	CG2	THR			10.657	34.838	35.539		37.17	6
	43	ATOM	114	C	THR			13.211	34.118	34.304		39.84	6
		ATOM		0	THR			13.796	33.796	35.365		40.55	8
		ATOM	115		PRO			13.055	33.261	33.288		38.20	7
		ATOM	116	N	PRO			12.370	33.534	32.023		36.34	6
		ATOM	117	CD				13.595	31.894	33.363		36.63	6
	50	ATOM	118	CA	PRO PRO			13.153	31.244	32.064		32.95	6
		ATOM	119	CB				12.573	32.291	31.239		35.75	6
		ATOM	120	CG	PRO				31.932	33.476		38.60	6
		ATOM	121	С	PRO			15.101		33.898		37.67	8
		ATOM	122	0	PRO			15.746	30.981 33.051	33.035		37.05	7
	55	ATOM	123	N	ALA			15.656	33.277	33.041		33.18	6
		ATOM	124	CA	ALA			17.087	34.599	32.348		30.56	6
		ATOM	125	CB	ALA			17.376 17.624	33.312	34.452		33.47	6
		ATOM	126	С	ALA	А	219	17.024	JJ.J12	24.422	1.00	55.47	

	5	ATOM	235	CB	PHE	Α	293	25.398	28.107	47.715	1.00	40.98	6
		ATOM	236	CG	PHE	Α	293	24.348	29.168	47.524	1.00	42.78	6
		ATOM	237	CD1	PHE	Α	293	24.654	30.493	47.747	1.00	44.40	6
		ATOM	238		PHE			23.071	28.833	47.116	1.00	43.66	6
		ATOM	239	CE1	PHE	Α	293	23.701	31.478	47.564	1.00	39.83	6
	10	ATOM	240		PHE			22.112	29.819	46.930	1.00	46.21	6
		ATOM	241	CZ	PHE			22.430	31.146	47.155	1.00	45.18	6
		ATOM	242	С	PHE			24.979	27.772	50.164	1.00	45.54	6
		ATOM	243	ō	PHE			24.686	28.576	51.034	1.00	42.01	8
		ATOM	244	N	CYS			24.426	26.572	50.062	1.00	47.05	7
	15	ATOM	245	CA	CYS			23.386	26.125	50.962	1.00	50.15	6
	15	ATOM	246	СВ	CYS			22.944	24.733	50.524	1.00	45.90	6
		ATOM	247	SG	CYS			22.303	24.663	48.829	1.00	51.50	16
		ATOM	248	C	CYS			23.825	26.125	52.423	1.00	51.38	6
		ATOM	249	0	CYS			23.008	25.954	53.322		53.83	8
	20	ATOM	250	N	GLU			25.119	26.327	52.645		49.72	7
	20	ATOM	251	CA	GLU			25.666	26.384	53.996		52.53	6
		ATOM	252	CB	GLU			27.103	25.830	54.015		57.40	6
		ATOM	253	CG	GLU			27.182	24.309	54.061		69.63	6
D		ATOM	254	CD	GLU			26.660	23.747	55.342		78.49	6
	25	ATOM	255		GLU			27.291	23.946	56.412		82.82	8
IU	23	ATOM	256		GLU			25.590	23.086	55.335		85.30	8
10		ATOM	257	C	GLU			25.653	27.831	54.488		48.54	6
losi-		ATOM	258	0	GLU			26.365	28.184	55.426		49.82	8
aj.		ATOM	259	N	LEU			24.804	28.631	53.846		43.79	7
lut.	30	ATOM	260	CA	LEU			24.670	30.034	54.159		45.42	6
300	50	ATOM	261	CB	LEU			25.062	30.864	52.923		41.04	6
21		ATOM	262	CG	LEU			26.438	30.658	52.315		42.74	6
E Pri		ATOM	263		LEU			26.447	31.030	50.861		40.99	6
Ш		ATOM	264		LEU			27.437	31.454	53.086		39.44	6
1 he	35	ATOM	265	C	LEU			23.239	30.366	54.548		45.56	6
A sour	55	ATOM	266	ō	LEU			22.301	29.660	54.148	1.00	43.07	8
· D		ATOM	267	N	PRO			23.050	31.405	55.365	1.00	46.99	7
Ü		ATOM	268	CD	PRO			24.121	32.241	55.930	1.00	47.12	6
		ATOM	269	CA	PRO			21.700	31.811	55.787	1.00	49.61	6
	40	ATOM	270	СВ	PRO			21.937	32.990	56.738	1.00	49.91	6
		ATOM	271	CG			297	23.401	33.155	56.872	1.00	51.28	6
		ATOM	272	С			297	20.864	32.212	54.558	1.00	49.59	6
		ATOM	273	0			297	21.402	32.684	53.556	1.00	51.66	8
		ATOM	274	N			298	19.545	32.035	54.655	1.00	51.02	7
	45	ATOM	275	CA			298	18.618	32.369	53.567	1.00	52.86	6
		ATOM	276	СВ			298	17.201	31.877	53.915	1.00	54.57	6
		ATOM	277	SG			298	16.040	33.162	54.440	1.00	67.87	16
		ATOM	278	c			298	18.583	33.863	53.291	1.00	48.51	6
		ATOM	279	ō			298	18.039	34.288	52.282	1.00	49.58	8
	50	ATOM	280	N			299	19.144	34.654	54.202		44.17	7
	50	ATOM	281	CA			299	19.179	36.096	54.016	1.00	47.57	6
		ATOM	282	CB			299	19.265	36.833	55.360	1.00	49.92	6
		ATOM	283	CG			299	17.931	36.996	56.125		59.30	6
		ATOM	284	CD			299	17.613	35.904	57.095		63.80	6
	55	ATOM	285	OE1			299	16.512	35.952	57.706		69.03	8
	55	ATOM	286	OE2			299	18.436	34.976	57.292		67.10	8
		ATOM	287	C			299	20.359	36.492	53.152		46.57	6
		ATOM	288	0			299	20.265	37.441	52.379		44.65	8
			200	~					_				

	5	ATOM	289	N	ASP	Α	300	21.467	35.765	53.294	1.00	45.17	7
		ATOM	290	CA	ASP	Α	300	22.661	36.042	52.509	1.00	43.32	6
		ATOM	291	CB	ASP	Α	300	23.919	35.513	53.213	1.00	37.38	6
		ATOM	292	CG	ASP	Α	300	24.223	36.239	54.473	1.00	36.23	6
		ATOM	293	OD1	ASP	Α	300	24.153	37.488	54.493	1.00	35.87	8
	10	ATOM	294	OD2	ASP	Α	300	24.572	35.575	55.483	1.00	40.14	8
		ATOM	295	С	ASP	Α	300	22.514	35.390	51.138	1.00	42.81	6
		ATOM	296	0	ASP			22.775	36.021	50.113	1.00	46.02	8
		ATOM	297	N	GLN			22.095	34.124	51.137		38.60	7
		ATOM	298	CA	GLN			21.896	33.390	49.902	1.00	40.00	6
	15	ATOM	299	CB	GLN			20.991	32.179	50.137	1.00	38.59	6
	10	ATOM	300	CG	GLN			21.644	31.003	50.808		40.26	6
		ATOM	301	CD	GLN			20.690	29.824	50.988	1.00	44.15	6
		ATOM	302	OE1	GLN			19.658	29.957	51.675	1.00	45.73	8
		ATOM	303	NE2	GLN			21.027	28.685	50.394		46.13	7
	20	ATOM	304	С	GLN			21.242	34.305	48.877		41.64	6
	20	ATOM	305	0	GLN			21.482	34.185	47.686		45.02	8
		ATOM	306	N			302	20.413	35.228	49.372		41.01	7
		ATOM	307	CA			302	19.726	36.179	48.511		40.23	6
34	100	ATOM	308	CB			302	18.502	36.774	49.217		39.52	6
1	25	ATOM	309	CG2	ILE			17.818	37.788	48.342		31.98	6
1	3 23	ATOM	310	CG1	ILE			17.502	35.673	49.581		40.77	6
5	e A	ATOM	311	CD1	ILE			17.003	34.897	48.385		45.43	6
£.,		ATOM	312	C			302	20.698	37.268	48.096		38.58	6
÷2,			313	0			302	20.960	37.453	46.906		40.81	8
4		ATOM	314	N			303	21.228	37.972	49.097		37.50	7
1		ATOM	315	CA	ILE		303	22.179	39.060	48.874		39.33	6
11		ATOM	316	CB			303	23.023	39.338	50.109		39.06	6
#n	3	ATOM	317		ILE			23.946	40.522	49.861		36.19	6
1		ATOM		CG1	ILE			22.141	39.653	51.313		40.15	6
1,3	1 25	ATOM	318 319		ILE			22.141	39.806	52.589		36.93	6
1 m	33	ATOM		CDI			303	23.093	38.705	47.722		36.49	6
19	3	ATOM	320 321	0			303	23.354	39.509	46.835		36.58	8
1.0	j	ATOM					304	23.580	37.477	47.762		32.91	7
		ATOM	322 323	N CA			304	24.465	36.964	46.734		27.55	6
	40	ATOM		CB			304	24.405	35.554	47.123		22.35	6
	40	MOTA	324 325	CG			304	26.150	35.480	48.029		26.88	6
		ATOM	326	CD1	LEU			26.267	36.731	48.876		24.82	6
		ATOM	327		LEU			26.084	34.226	48.861		23.69	6
		ATOM	328	CDZ			304	23.764	36.968	45.389		28.05	6
	45	ATOM	329	0			304	24.212	37.623	44.443		24.68	8
	43	MOTA					305	22.657	36.236	45.318		26.34	7
		ATOM	330	N				21.892	36.147	44.089		30.91	6
		ATOM	331	CA			305	20.565	35.434	44.359		32.50	6
		ATOM	332	CB			305			44.635		33.36	6
	50	ATOM	333	CG			305	20.637	33.950 33.370	44.033		33.87	6
	50	ATOM	334		LEU			19.247		43.466		31.72	6
		ATOM	335		LEU			21.340	33.280	43.477		29.76	6
		ATOM	336	С			305	21.665	37.524 37.747	42.301		29.33	8
		ATOM	337	0			305	21.954				29.72	7
		ATOM	338	N			306	21.157	38.439	44.298		34.28	6
	55	ATOM	339	CA			306	20.868	39.800	43.864		35.98	6
		ATOM	340	CB			306	20.293	40.615	45.026		43.35	6
		ATOM	341	CG	LYS			18.919	40.163	45.511 46.559		51.50	6
		ATOM	342	CD	LIS	А	306	18.397	41.127	40.009	1.00	51.50	Ü

	5	ATOM	397	CA	SER	Α	314	26.005	38.472	31.197		27.98	6
		ATOM	398	CB	SER	Α	314	26.354	39.914	31.581	1.00	29.64	6
		ATOM	399	OG	SER	Α	314	26.956	39.972	32.858	1.00	43.44	8
		ATOM	400	С	SER	Α	314	27.275	37.679	30.851	1.00	22.30	6
		ATOM	401	0	SER	Α	314	27.675	37.629	29.690	1.00	24.18	8
	10	ATOM	402	N	LEU	А	315	27.905	37.048	31.845	1.00	23.99	7
		ATOM	403	CA	LEU			29.099	36.261	31.563	1.00	25.07	6
		ATOM	404	CB	LEU			29.685	35.593	32.816		19.11	6
		ATOM	405	CG	LEU			30.675	34.479	32.505		20.39	6
		ATOM	405		LEU			31.866	35.040	31.756		18.92	6
	15		407		LEU			31.125	33.789	33.765		12.93	6
	13	ATOM						28.700	35.180	30.597		24.53	6
		MOTA	408	C	LEU				35.036	29.556		26.32	8
		ATOM	409	0	LEU			29.304				28.18	7
		ATOM	410	N	ARG			27.678	34.426	30.982			6
		ATOM	411	CA	ARG			27.151	33.312	30.216		27.54	
	20	ATOM	412	CB	ARG			25.915	32.752	30.928		27.39	6
		MOTA	413	CG	ARG			26.188	32.190	32.336		22.00	6
		ATOM	414	CD	ARG			24.934	31.526	32.901		18.78	6
		ATOM	415	NE	ARG			25.245	30.376	33.721		26.57	7
13		ATOM	416	CZ	ARG	Α	316	24.341	29.468	34.054		30.81	6
40	25	ATOM	417	NH1	ARG	Α	316	23.084	29.614	33.639		33.71	7
IU		ATOM	418	NH2	ARG	Α	316	24.701	28.416	34.776		33.13	7
110		ATOM	419	С	ARG	Α	316	26.774	33.660	28.794		28.09	6
Į:mh		ATOM	420	0	ARG	Α	316	26.737	32.792	27.931	1.00	32.41	8
14		ATOM	421	N	ALA	Α	317	26.484	34.936	28.571	1.00	28.36	7
Ende	30	ATOM	422	CA	ALA	Α	317	26.094	35.411	27.264	1.00	26.64	6
143		ATOM	423	CB	ALA	Α	317	25.232	36.666	27.418	1.00	22.93	6
51		ATOM	424	С	ALA	Α	317	27.323	35.714	26.417	1.00	28.35	6
(3)		ATOM	425	0	ALA	Α	317	27.398	35.342	25.252	1.00	32.10	8
14		MOTA	426	N	ALA	А	318	28.286	36.396	27.026	1.00	29.12	7
U	35	ATOM	427	CA	ALA			29.515	36.760	26.350	1.00	27.50	6
list		ATOM	428	CB	ALA			30.434	37.452	27.333	1.00	28.39	6
÷Ū		ATOM	429	С	ALA			30.181	35.502	25.825	1.00	28.10	6
10		ATOM	430	0	ALA			30.600	35.447	24.678	1.00	28.18	8
		ATOM	431	N	VAL			30.255	34.491	26.700	1.00	29.16	7
	40	ATOM	432	CA	VAL			30.880	33.198	26.393		35.24	6
	-10	ATOM	433	CB	VAL			30.703	32.210	27.547		27.34	6
		ATOM	434		VAL			30.895	32.891	28.858		29.96	6
		ATOM	435		VAL			29.353	31.552	27.482		31.70	6
		ATOM	436	C			319	30.215	32.608	25.165		40.01	6
	45	ATOM	437	0			319	30.640	31.575	24.680		42.70	8
	43			N	ARG			29.176	33.284	24.683		38.64	7
		ATOM	438		ARG			28.415	32.822	23.545		38.61	6
		ATOM	439	CA				27.031	32.458	24.043		37.26	6
		ATOM	440	CB			320					43.12	6
		ATOM	441	CG			320	26.863	30.991	24.192		50.79	6
	50	ATOM	442	CD	ARG			25.637	30.642	25.014			7
		ATOM	443	NE			320	25.258	29.256	24.770		54.71	
		ATOM	444	CZ	ARG			24.331	28.625	25.501		57.89	6
		MOTA	445		ARG			23.667	29.291	26.440		49.08	7
		ATOM	446		ARG			23.964	27.385	25.242		59.59	7
	55	ATOM	447	С			320	28.292	33.825	22.405		42.14	6
		ATOM	448	0			320	27.251	33.909	21.748		46.30	8
		ATOM	449	N			321	29.352	34.583	22.173		42.04	7
		ATOM	450	CA	TYR	Α	321	29.366	35.555	21.098	1.00	42.70	6

	5	ATOM	451	CB	TYR 2	A	321	30.083	36.810	21.575		38.01	6
		ATOM	452	CG	TYR 2	Α	321	30.601	37.650	20.448	1.00	37.94	6
		ATOM	453	CD1	TYR 2	Α	321	29.733	38.296	19.574	1.00	33.85	6
		ATOM	454	CE1	TYR 2	A	321	30.235	39.037	18.494	1.00	34.49	6
		ATOM	455		TYR 2			31.966	37.743	20.224	1.00	28.03	6
	10	ATOM	456		TYR			32.473	38.475	19.153		32.69	6
	10	ATOM	457	CZ	TYR			31.612	39.125	18.276		35.18	6
		ATOM	458	OH	TYR			32.107	39.866	17.223		39.48	8
		ATOM	459	C	TYR .			30.085	35.005	19.877		45.51	6
				0	TYR .			31.261	34.697	19.951		48.02	8
	1.5	ATOM	460					29.354	34.879	18.773		44.56	7
	15	MOTA	461	N	ASP .					17.502		45.86	6
		MOTA	462	CA	ASP .			29.912	34.400			46.64	6
		MOTA	463	CB	ASP .			28.804	33.670	16.736			
		ATOM	464	CG	ASP .			29.050	33.608	15.255		40.00	6
		ATOM	465		ASP .			30.010	34.256	14.768		40.00	8
	20	MOTA	466		ASP .			28.262	32.929	14.536		40.00	8
		ATOM	467	С	ASP .			30.460	35.629	16.755		45.82	6
		ATOM	468	0	ASP .	A	322	29.678	36.464	16.271		45.38	8
		ATOM	469	N	PRO .	Α	323	31.800	35.735	16.584		46.53	7
8		ATOM	470	CD	PRO .	Α	323	32.774	34.719	16.991	1.00	47.16	6
	□ 25	ATOM	471	CA	PRO .	A	323	32.424	36.889	15.890	1.00	46.63	6
- 5	U	ATOM	472	CB	PRO .	Α	323	33.921	36.603	15.936	1.00	43.95	6
i,	ġ.	ATOM	473	CG	PRO .	Α	323	34.099	35.303	16.582	1.00	43.93	6
1	sh	ATOM	474	C	PRO .	Α	323	31.953	37.087	14.453	1.00	48.34	6
	4	ATOM	475	ō	PRO			31.797	38.210	13.960	1.00	50.84	8
1	··· 30	ATOM	476	N	GLU			31.778	35.970	13.752	1.00	52.39	7
	ų Jo	ATOM	477	CA	GLU			31.339	35.968	12.370	1.00	55.85	6
31		ATOM	478	CB	GLU			31.035	34.528	11.965		55.54	6
ť.	3	ATOM	479	CG	GLU			32.224	33.584	12.104		40.00	6
197	i.l	ATOM	480	CD	GLU		324	33.432	34.023	11.310		40.00	6
Ž.	35	ATOM	481	OE1	GLU			33.350	35.040	10.555		40.00	8
1	1 33		482	OE2	GLU			34.506	33.356	11.415		40.00	8
9	0	ATOM		C	GLU			30.077	36.798	12.277		54.94	6
*	Ç .	ATOM	483		GLU			30.077	37.892	11.730		59.81	8
		ATOM	484	0					36.212	12.810		52.95	7
	40	MOTA	485	N	SER		325	29.009		12.839		50.10	6
	40	ATOM	486	CA	SER			27.695	36.812	13.402		48.23	6
		MOTA	487	CB	SER			26.701	35.797				8
		MOTA	488	OG	SER			27.183	35.239	14.615		48.71	6
		ATOM	489	С	SER			27.651	38.093	13.659		50.61	
		ATOM	490	0	SER			26.885	38.992	13.354		52.19	8
	45	ATOM	491	N	GLU			28.495	38.168	14.687		45.64	7
		ATOM	492	CA	GLU			28.567	39.341	15.546		43.35	6
		ATOM	493	CB	GLU	Α	326	28.830	40.608	14.711		42.74	6
		ATOM	494	CG	GLU	Α	326	30.148	40.606	13.945		50.32	6
		ATOM	495	CD	GLU	Α	326	30.451	41.925	13.313		56.34	6
	50	ATOM	496	OE1	GLU	Α	326	31.509	42.046	12.649		59.31	8
		ATOM	497	OE2	GLU	Α	326	29.656	42.890	13.452	1.00	55.74	8
		ATOM	498	С	GLU	Α	326	27.288	39.526	16.340	1.00	40.23	6
		ATOM	499	0	GLU	Α	326	26.695	40.603	16.340	1.00	40.44	8
		ATOM	500	N	THR			26.888	38.474	17.051	1.00	35.90	7
	55	ATOM	501	CA	THR			25.663	38.506	17.860	1.00	37.29	6
		ATOM	502	СВ	THR			24.466	38.057	17.024	1.00	37.63	6
		ATOM	503	OG1				24.661	36.709	16.580	1.00	38.12	8
		ATOM	504		THR			24.269	38.965	15.810	1.00	39.90	6
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	5	ATOM	613	CG	LYS	Α	342	23.655	50.536	23.240	1.00	40.00	6
		ATOM	614	CD	LYS	Α	342	24.673	51.109	22.245	1.00	34.48	6
		ATOM	615	CE	LYS	Α	342	25.514	52.229	22.873	1.00		6
		ATOM	616	NZ	LYS	A	342	26.655	52.634	21.987	1.00	42.32	7
		ATOM	617	C	LYS	Α	342	20.796	49.349	23.774	1.00	38.29	8
	10	ATOM	618	0	LYS	Α	342	20.345	49.711	24.861	1.00	36.23	8
		ATOM	619	N	ASN	Α	343	20.223	49.622	22.603	1.00	39.25	7
		ATOM	620	CA	ASN	Α	343	18.993	50.385	22.485	1.00	40.19	6
		ATOM	621	CB	ASN	Α	343	18.521	50.373	21.033	1.00	37.96	6
		ATOM	622	CG	ASN	Α	343	19.664	50.550	20.052	1.00	39.22	6
	15	ATOM	623	OD1	ASN	Α	343	20.428	51.537	20.125	1.00	42.37	8
		ATOM	624	ND2	ASN	Α	343	19.773	49.612	19.125	1.00	42.19	7
		ATOM	625	С	ASN	Α	343	17.928	49.748	23.375	1.00	40.12	6
		ATOM	626	0	ASN	Α	343	17.010	50.417	23.859	1.00	36.01	8
		ATOM	627	N	GLY			18.073	48.433	23.568	1.00	40.95	7
	20	ATOM	628	CA	GLY			17.152	47.670	24.394	1.00	39.25	6
		ATOM	629	С	GLY			17.039	48.092	25.842	1.00	38.26	6
		ATOM	630	0	GLY	Α	344	16.072	47.724	26.512	1.00	35.69	8
		ATOM	631	N	GLY	Α	345	18.017	48.857	26.329	1.00	35.89	7
(3		ATOM	632	CA	GLY	Α	345	17.964	49.301	27.706	1.00	34.00	6
·D	25	ATOM	633	С	GLY	А	345	19.273	49.199	28.443	1.00	38.64	6
171		ATOM	634	0	GLY			19.469	49.888	29.441	1.00	38.14	8
10		ATOM	635	N	LEU	Α	346	20.170	48.337	27.973	1.00	39.52	7
Ink		ATOM	636	CA	LEU			21.444	48.180	28.649	1.00	36.05	6
Bugg		ATOM	637	CB	LEU	Α	346	22.124	46.876	28.209	1.00	35.72	6
fieb.	30	ATOM	638	CG	LEU	Α	346	21.355	45.617	28.501	1.00	34.89	6
1.1		ATOM	639	CD1	LEU	Α	346	22.295	44.413	28.422	1.00	44.09	6
10		ATOM	640	CD2	LEU	Α	346	20.786	45.721	29.902	1.00	34.84	6
120		ATOM	641	C	LEU	Α	346	22.358	49.361	28.396	1.00	33.52	6
1,1,1		ATOM	642	0	LEU	Α	346	23.267	49.653	29.178	1.00	35.58	8
1,1	35	ATOM	643	N	GLY	Α	347	22.087	50.056	27.295	1.00	30.47	7
Trad		ATOM	644	CA	GLY	Α	347	22.909	51.192	26.931	1.00	33.01	6
10		ATOM	645	С	GLY	Α	347	24.360	50.768	26.747	1.00	30.72	6
G		ATOM	646	0	GLY	Α	347	24.669	49.775	26.082	1.00	30.89	8
		ATOM	647	N	VAL	Α	348	25.244	51.556	27.355	1.00	31.30	7
	40	ATOM	648	CA	VAL	Α	348	26.671	51.325	27.286		31.27	6
		ATOM	649	CB	VAL	Α	348	27.441	52.294	28.184		31.66	6
		ATOM	650	CG1	VAL	Α	348	27.067	52.107	29.631		20.19	6
		MOTA	651	CG2	VAL	Α	348	28.931	52.138	27.986		24.77	6
		ATOM	652	С	VAL	Α	348	27.063	49.892	27.678		33.84	6
	45	MOTA	653	0	VAL	Α	348	28.095	49.392	27.225		29.99	8
		MOTA	654	N	VAL			26.253	49.227	28.514		33.31	7
		ATOM	655	CA	VAL	А	349	26.568	47.881	28.906		32.23	6
		ATOM	656	CB	VAL	Α	349	25.581	47.259	29.858		32.59	6
		ATOM	657	CG1	VAL	Α	349	25.865	45.795	29.985		33.68	6
	50	ATOM	658	CG2	VAL	Α	349	25.687	47.899	31.213		32.30	6
		ATOM	659	С	VAL	Α	349	26.706	46.985	27.726		34.91	6
		MOTA	660	0	VAL	Α	349	27.583	46.136	27.735		33.73	8
		ATOM	661	N	SER	Α	350	25.875	47.134	26.702		32.81	7
		ATOM	662	CA	SER	Α	350	26.001	46.252	25.556	1.00	30.10	6
	55	ATOM	663	CB	SER			25.119	46.665	24.411		24.95	6
		MOTA	664	OG			350	25.209	45.675	23.394		23.16	8
		MOTA	665	С	SER	Α	350	27.445	46.257	25.129		31.59	6
		ATOM	666	0	SER	Α	350	28.116	45.244	25.284	1.00	37.62	8

5	ATOM	721	СВ	MET	Α	358	3	5.143	40.606	21.009	1.00	34.56	6
	ATOM	722	CG	MET	Α	358	3	3.949	41.145	20.290	1.00	46.43	6
	ATOM	723	SD	MET	А	358	3	4.207	42.776	19.514	1.00	42.13	16
	ATOM	724	CE	MET	Α	358	3	4.507	43.855	20.994	1.00	44.29	6
	ATOM	725	С	MET				6.256	38.762	22.230	1.00	33.26	6
10	ATOM	726	0	MET		358	3	6.894	37.807	21.795	1.00	36.39	8
	ATOM	727	N	SER			3	6.637	39.491	23.281	1.00	33.31	7
	ATOM	728	CA	SER				7.860	39.226	24.019	1.00	34.39	6
	ATOM	729	CB	SER				7.869	40.067	25.295	1.00	30.84	6
	ATOM	730	OG	SER				9.135	40.008	25.930		47.14	8
15	ATOM	731	C	SER				7.984	37.748	24.357		36.43	6
	ATOM	732	o	SER				8.900	37.078	23.896		35.46	8
	ATOM	733	N	LEU				7.046	37.264	25.166		36.74	7
	ATOM	734	CA	LEU		360		7.017	35.875	25.604		35.44	6
	ATOM	735	CB	LEU		360		5.708	35.579	26.336		34.16	6
20	ATOM	736	CG	LEU				5.471	36.290	27.644		34.59	6
20	ATOM	737	CD1	LEU		360		4.225	35.765	28.312		33.53	6
	ATOM	738	CD2	LEU				6.658	36.052	28.541		31.69	6
	ATOM	739	CDZ	LEU				7.203	34.862	24.500		38.72	6
2754	ATOM	740	0	LEU				7.820	33.828	24.728		38.29	8
(I)		741	N	SER				6.635	35.147	23.328		40.96	7
1页 25	ATOM	741	CA	SER				6.777	34.262	22.186		45.67	6
iu iu	ATOM					361		6.518	35.045	20.904		46.45	6
List Indi	ATOM	743	CB					5.210	35.598	20.904		51.81	8
14	ATOM	744	OG	SER					33.627	22.145		44.49	6
	ATOM	745	C			361		8.166		21.625		46.67	8
30	ATOM	746	0	SER				8.347	32.538	22.703		41.44	7
ii.	ATOM	747	N			362		9.134	34.348	22.703		42.13	6
free?	ATOM	748	CA			362		0.525	33.918			42.13	6
W	MOTA	749	CB			362		1.408	35.131	23.066		51.87	8
5.4	ATOM	750	OG			362		1.219	36.136			38.41	6
35	ATOM	751	C			362		0.798	32.870	23.876		38.01	8
-D	ATOM	752	0			362		1.553	31.938	23.641		34.55	7
ID.	ATOM	753	N	PHE		363		0.198	33.039	25.058		32.96	6
	MOTA	754	CA			363		0.417	32.126	26.174		31.99	6
40	MOTA	755	CB			363		9.832	32.718	27.447		29.97	6
40	ATOM	756	CG	PHE		363		0.448	34.036	27.840		30.61	6
	MOTA	757		PHE				0.102	34.650	29.020 27.014		32.02	6
	ATOM	758		PHE		363		1.379	34.646			33.67	6
	ATOM	759	CE1			363		0.685	35.856	29.391 27.377		30.91	6
4.5	ATOM	760		PHE				1.959	35.843			29.33	6
45	ATOM	761	CZ	PHE		363		1.615	36.456	28.558			
	ATOM	762	С			363		9.883	30.716	25.967		30.52	6
	ATOM	763	0			363		0.436	29.766	26.526		32.19	8
	ATOM	764	N			364		8.817	30.570	25.175		33.51	7
	ATOM	765	CA			364		8.239	29.264	24.918		38.03	6
50	ATOM	766	CB	ASN				9.240	28.404	24.139		42.32	6
	ATOM	767	CG			364		9.696	29.065	22.861		53.11	6
	ATOM	768		ASN				8.874	29.330	21.954		59.51	8
	ATOM	769		ASN		364		0.986	29.330	22.772		55.95	7
	ATOM	770	С			364		7.916	28.572	26.235		31.89	6
55	ATOM	771	0			364		8.324	27.428	26.457		30.28	8
	ATOM	772	N			365		7.176	29.271	27.094		27.62	7
	MOTA	773	CA			365		6.806	28.743	28.406		29.36	6
	ATOM	774	CB	LEU	А	365	3	6.195	29.866	29.237	1.00	27.54	6

	5	ATOM	775	CG	LEU	Α	365	36.990	31.150	29.185	1.00 38	.91	6
		ATOM	776	CD1	LEU	Α	365	36.316	32.216	30.036	1.00 34	. 47	6
		ATOM	777		LEU			38.406	30.883	29.663	1.00 34	.24	6
		ATOM	778	C	LEU			35.830	27.590	28.262	1.00 26	.23	6
		ATOM	779	ō	LEU			34.890	27.649	27.472	1.00 27		8
	10										1.00 27		7
	10	ATOM	780	N	ASP			36.083	26.528	29.021			
		MOTA	781	CA	ASP			35.213	25.358	28.988	1.00 26		6
		ATOM	782	CB	ASP	Α	366	36.027	24.049	29.033	1.00 29		6
		ATOM	783	CG	ASP	Α	366	36.799	23.874	30.303	1.00 35	.74	6
		ATOM	784	OD1	ASP	Α	366	36.285	24.177	31.402	1.00 36	.78	8
	15	ATOM	785	OD2	ASP	Α	366	37.959	23.386	30.240	1.00 41	.23	8
		ATOM	786	С	ASP			34.278	25.434	30.181	1.00 27	.70	6
		MOTA	787	ō	ASP			34.587	26.097	31.173	1.00 31		8
		ATOM	788	N	ASP			33.141	24.743	30.066	1.00 29		7
		ATOM	789	CA	ASP			32.120	24.679	31.120	1.00 32		6
	20				ASP			31.472	23.284	31.120	1.00 38		6
	20	ATOM	790	CB							1.00 38		6
		ATOM	791	CG	ASP			30.806	22.924	29.854			
		ATOM	792		ASP			29.877	23.650	29.409	1.00 35		8
		ATOM	793		ASP			31.186	21.884	29.250	1.00 51		8
1000		ATOM	794	C	ASP			32.754	24.969	32.482	1.00 33		6
·Ø	25	ATOM	795	0	ASP			32.484	26.000	33.098	1.00 38		8
FU		MOTA	796	N	THR	Α	368	33.602	24.032	32.919	1.00 31		7
10		ATOM	797	CA	THR	Α	368	34.329	24.124	34.181	1.00 26	.28	6
garnes.		ATOM	798	CB	THR	Α	368	35.559	23.222	34.141	1.00 27	.30	6
4		ATOM	799	OG1	THR	Α	368	35.161	21.871	33.885	1.00 33	.42	8
in the	30	ATOM	800	CG2	THR			36.323	23.303	35.454	1.00 25	.16	6
1		ATOM	801	С	THR			34.764	25.557	34.479	1.00 21	.13	6
98		ATOM	802	0	THR			34.408	26.153	35.503	1.00 23		8
100		ATOM	803	N	GLU			35.545	26.092	33.551	1.00 21		7
Li		ATOM	804	CA	GLU			36.065	27.435	33.661	1.00 28		6
	35		805	CB	GLU			36.960	27.707	32.453	1.00 32		6
Ü	33	MOTA			GLU			38.089	26.663	32.346	1.00 36		6
453		MOTA	806	CG						31.110	1.00 30		6
175		ATOM	807	CD	GLU			38.906	26.747				
		ATOM	808		GLU			38.337	26.744	29.994	1.00 42		8
		ATOM	809		GLU			40.158	26.795	31.218	1.00 42		8
	40	ATOM	810	С	GLU			34.953	28.471	33.821	1.00 25		6
		ATOM	811	0	GLU			34.987	29.256	34.760	1.00 20		8
		MOTA	812	N	VAL			33.967	28.463	32.921	1.00 25		7
		ATOM	813	CA	VAL	Α	370	32.849	29.396	33.029	1.00 25		6
		MOTA	814	CB	VAL	Α	370	31.763	29.131	31.987	1.00 26	.15	6
	45	ATOM	815	CG1	VAL	Α	370	30.609	30.093	32.183	1.00 27	. 65	6
		ATOM	816	CG2	VAL	Α	370	32.306	29.251	30.592	1.00 17	.70	6
		ATOM	817	С	VAL	Α	370	32.245	29.209	34.412	1.00 26	.49	6
		ATOM	818	0	VAL			32.012	30.170	35.147	1.00 28	.16	8
		ATOM	819	N	ALA			31.988	27.947	34.739	1.00 21	.01	7
	50	ATOM	820	CA	ALA			31.393	27.554	36.011	1.00 19		6
	50	ATOM	821	CB	ALA			31.441	26.039	36.145	1.00 18		6
			822	C	ALA			32.116	28.211	37.177	1.00 23		6
		ATOM							28.989	37.931	1.00 23		8
		ATOM	823	0	ALA			31.531					
		ATOM	824	N	LEU			33.401	27.893	37.305	1.00 22		7 6
	55	ATOM	825	CA	LEU		372	34.217	28.447	38.369	1.00 23		
		MOTA	826	CB	LEU			35.675	27.996	38.178	1.00 27		6
		ATOM	827	CG	LEU			35.943	26.524	38.415	1.00 21		6
		MOTA	828	CD1	LEU	Α	372	37.356	26.171	38.049	1.00 27	.64	6

	5	ATOM	829		LEU			35.675 34.098	26.204 29.966	39.880 38.396		20.90 21.34	6 6
		ATOM	830	C	LEU								8
		ATOM	831	0	LEU			33.828	30.572	39.439		23.16	7
		ATOM	832	N	LEU			34.288 34.214	30.561	37.223 37.074		23.78	6
	10	ATOM	833	CA	LEU				32.007 32.360			22.18	6
	10	ATOM	834	CB	LEU			34.296		35.575			6
		ATOM	835	CG	LEU			34.784	33.726	35.165		31.52	
		ATOM	836		LEU			36.000	34.084	35.962		31.93	6
		ATOM	837		LEU			35.103	33.720	33.693		30.24	6
		ATOM	838	С	LEU			32.904	32.480	37.720		25.69	6
	15	ATOM	839	0	LEU			32.895	33.410	38.532		30.13	8
		ATOM	840	N	GLN			31.814	31.800	37.368		26.24	7
		ATOM	841	CA	GLN			30.487	32.104	37.896		21.60	6
		ATOM	842	CB	GLN		374	29.454	31.121	37.335		24.57	6
		ATOM	843	CG	GLN			29.310	31.145	35.821		21.02	6
	20	ATOM	844	CD	GLN			28.224	30.201	35.331		22.86	6
		ATOM	845	OE1	GLN			28.037	30.042	34.123		24.07	8
		ATOM	846		GLN			27.515	29.590	36.249		25.59	7
		ATOM	847	C	GLN			30.421	32.039	39.422		20.66	6
100		ATOM	848	0	GLN			29.717	32.832	40.048		24.47	8
10	25	ATOM	849	N	ALA			31.136	31.074	40.004		16.26	7
T		ATOM	850	CA	ALA			31.155	30.889	41.445		17.16	6
(11)		ATOM	851	CB	ALA			31.805	29.568	41.780		19.53	6
1.4		ATOM	852	С	ALA	Α	375	31.907	32.025	42.108		25.13	6
114		ATOM	853	0	ALA	Α	375	31.397	32.646	43.034		23.81	8
ech.	30	MOTA	854	N	VAL	А	376	33.122	32.277	41.611		24.57	7
- Sales		ATOM	855	CA	VAL	А	376	33.959	33.354	42.118		25.80	6
5! Jess		ATOM	856	CB	VAL	Α	376	35.101	33.658	41.164		26.48	6
100		ATOM	857	CG1	VAL	А	376	35.926	34.812	41.697		23.20	6
(4)		MOTA	858	CG2	VAL		376	35.959	32.429	40.952		19.08	6
N	35	ATOM	859	С	VAL			33.107	34.599	42.312		25.69	6
40		ATOM	860	0	VAL	Α	376	33.297	35.364	43.251		27.87	8
10		ATOM	861	N	LEU			32.159	34.781	41.399		23.09	7
1968		ATOM	862	CA	LEU			31.242	35.915	41.423		22.86	6
		ATOM	863	CB	LEU			30.540	36.031	40.061		18.50	6
	40	MOTA	864	CG	LEU			31.424	36.368	38.885		22.65	6
		ATOM	865		LEU			30.689	36.227	37.601		16.70	6
		ATOM	866	CD2	LEU			31.916	37.776	39.051		19.58	6
		ATOM	867	С	LEU			30.228	35.719	42.543		26.14	6
		ATOM	868	0	LEU			30.131	36.532	43.452		20.62	8
	45	ATOM	869	N	LEU			29.483	34.614	42.468		28.99	7
		ATOM	870	CA	LEU			28.469	34.303	43.475		28.87	6
		ATOM	871	CB	LEU			28.053	32.826	43.397		26.89	6
		ATOM	872	CG	LEU			27.110	32.344	44.472		28.83	6
		MOTA	873	CDI	LEU	Α	378	25.915	33.252	44.525		27.97	6
	50	ATOM	874	CD2	LEU	Α	378	26.693	30.928	44.205		27.69	6
		ATOM	875	С	LEU	Α	378	28.992	34.617	44.853		31.09	6
		ATOM	876	0	LEU	Α	378	28.399	35.421	45.573		31.77	8
		ATOM	877	N	MET	Α	379	30.118	33.991	45.189	1.00	31.44	7
		ATOM	878	CA	MET			30.736	34.141	46.494		32.62	6
	55	ATOM	879	CB	MET			31.690	32.960	46.744		31.45	6
		ATOM	880	CG	MET			30.984	31.595	46.792		38.75	6
		ATOM	881	SD	MET			29.741	31.626	48.107		41.27	16
		ATOM	882	CE	MET	Α	379	28.896	30.036	47.851	1.00	35.68	6

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	5	ATOM	883	С	MET			31.485	35.448	46.727		33.72	6
		ATOM	884	0	MET	Α	379	32.567	35.450	47.305	1.00	36.29	8
		ATOM	885	N	SER	Α	380	30.889	36.555	46.315	1.00	34.49	7
		ATOM	886	CA	SER	Α	380	31.498	37.853	46.550	1.00	33.97	6
		ATOM	887	CB	SER			30.921	38.890	45.576	1.00	31.24	6
	10	ATOM	888	OG	SER			31.205	38.543	44.230	1.00	39.42	8
	10	ATOM	889	С	SER			31.179	38.239	47.992		39.69	6
								30.029	38.446	48.357		44.64	8
		MOTA	890	0	SER							41.04	7
		MOTA	891	N	SER			32.214	38.313	48.812			
		MOTA	892	CA	SER			32.060	38.640	50.216		44.91	6
	15	MOTA	893	CB	SER			33.324	38.234	50.951		44.50	6
		MOTA	894	OG	SER	Α	381	34.431	39.002	50.510		45.42	8
		ATOM	895	С	SER	Α	381	31.795	40.106	50.499	1.00	44.59	6
		ATOM	896	0	SER	Α	381	31.476	40.470	51.618	1.00	49.32	8
		ATOM	897	N	ASP	Α	382	31.939	40.942	49.486	1.00	43.75	7
	20	ATOM	898	CA	ASP	А	382	31.744	42.362	49.641	1.00	43.93	6
		ATOM	899	CB	ASP			32.673	43.111	48.677	1.00	48.39	6
		ATOM	900	CG	ASP			32.572	42.624	47.263	1.00	53.23	6
		ATOM	901		ASP			32.705	41.400	47.034		56.97	8
344		ATOM	902		ASP			32.358	43.454	46.333		58.91	8
	25		902	C	ASP			30.314	42.885	49.507		41.09	6
T.	23	MOTA								49.845		40.93	8
113		MOTA	904	0	ASP			30.048	44.036			42.63	7
9,424 \$266		MOTA	905	N	ARG			29.397	42.049	49.034			
N		MOTA	906	CA	ARG			28.036	42.485	48.876		43.32	6
garb.		MOTA	907	CB	ARG			27.138	41.332	48.443		42.31	6
14.3	30	ATOM	908	CG	ARG			27.651	40.399	47.352		40.83	6
		MOTA	909	CD	ARG	Α	383	27.586	40.954	45.925		38.09	6
85.		ATOM	910	NE	ARG	Α	383	27.768	39.878	44.975		37.33	7
		ATOM	911	CZ	ARG	Α	383	28.037	40.058	43.693		38.35	6
5-10		ATOM	912	NH1	ARG	Α	383	28.142	41.292	43.198	1.00	33.70	7
U	35	ATOM	913	NH2	ARG	Α	383	28.194	38.992	42.918	1.00	35.46	7
7:22 25.		ATOM	914	С	ARG			27.523	42.989	50.216	1.00	44.96	6
Ø		ATOM	915	0	ARG	А	383	27.744	42.344	51.260	1.00	45.60	8
·D		ATOM	916	N	PRO			26.852	44.144	50.223	1.00	45.33	7
		ATOM	917	CD	PRO		384	26.625	44.964	49.027	1.00	46.85	6
	40	ATOM	918	CA	PRO			26.298	44.738	51.446		47.37	6
	40	ATOM	919	CB	PRO			25.841	46.130	51.012		46.90	6
			920	CG	PRO			26.075	46.229	49.567		46.41	6
		ATOM		C			384	25.158	43.919	52.049		48.29	6
		ATOM	921					24.404	43.264	51.329		48.34	8
		ATOM	922	0			384			53.383		49.88	7
	45	ATOM	923	N	GLY			25.039	43.983				
		ATOM	924	CA			385	23.991	43.270	54.113		50.35	6
		ATOM	925	С			385	24.347	41.852	54.495		50.70	6
		ATOM	926	0			385	23.614	41.204	55.244		53.48	8
		ATOM	927	N	LEU	Α	386	25.466	41.371	53.955		49.04	7
	50	ATOM	928	CA	LEU	Α	386	25.901	40.017	54.215		50.53	6
		ATOM	929	CB	LEU	Α	386	27.224	39.751	53.492	1.00	45.17	6
		ATOM	930	CG	LEU	Α	386	27.152	39.592	51.993	1.00	48.26	6
		ATOM	931	CD1	LEU	Α	386	28.542	39.439	51.404	1.00	41.68	6
		ATOM	932		LEU			26.302	38.374	51.682	1.00	38.40	6
	55	ATOM	933	С			386	26.045	39.776	55.691	1.00	52.13	6
	55	ATOM	934	o			386	26.296	40.692	56.459		53.67	8
		ATOM	935	N			387	25.861	38.522	56.077		53.42	7
		ATOM	936	CA			387	25.976	38.129	57.470		56.01	6
		ATOM	220	CM	MUM	21	201	23.510	50.125	57.4.0	1.00		

	5	ATOM	937	CB	ALA	Α	387	24.802	37.234	57.854		56.47	6
		ATOM	938	C	ALA	Α	387	27.289	37.385	57.659		55.52	6
		ATOM	939	0	ALA	Α	387	28.275	37.940	58.134		53.75	8
		ATOM	940	N	CYS	Α	388	27.273	36.120	57.253		56.03	7
		ATOM	941	CA	CYS	Α	388	28.412	35.236	57.370		59.57	6
	10	ATOM	942	CB	CYS	Α	388	27.923	33.803	57.172	1.00	59.23	6
		ATOM	943	SG	CYS	Α	388	26.397	33.431	58.009	1.00	58.64	16
		ATOM	944	С	CYS	Α	388	29.482	35.581	56.328	1.00	62.18	6
		ATOM	945	0	CYS	Α	388	29.720	34.821	55.400	1.00	67.88	8
		ATOM	946	N	VAL	Α	389	30.110	36.747	56.495	1.00	60.78	7
	15	ATOM	947	CA	VAL	Α	389	31.173	37.212	55.590	1.00	57.70	6
		ATOM	948	CB	VAL	Α	389	31.740	38.567	56.024	1.00	57.09	6
		ATOM	949	CG1	VAL	Α	389	32.795	39.037	55.041	1.00	59.03	6
		ATOM	950	CG2	VAL	Α	389	30.640	39.598	56.171	1.00	53.98	6
		ATOM	951	С	VAL	Α	389	32.297	36.182	55.550	1.00	57.77	6
	20	ATOM	952	0	VAL	Α	389	32.358	35.336	54.662	1.00	60.94	8
		ATOM	953	N	ALA	Α	390	33.182	36.292	56.528	1.00	52.68	7
		ATOM	954	CA	ALA	Α	390	34.347	35.431	56.684	1.00	48.41	6
		ATOM	955	CB	ALA			34.703	35.321	58.185	1.00	45.19	6
ies		ATOM	956	С	ALA	Α	390	34.224	34.040	56.082	1.00	47.63	6
	25	ATOM	957	0	ALA	Α	390	35.107	33.597	55.348	1.00	51.95	8
100		ATOM	958	N	ARG	Α	391	33.117	33.366	56.391	1.00	47.11	7
10		ATOM	959	CA	ARG			32.879	32.018	55.885	1.00	51.64	6
146		ATOM	960	СВ	ARG			31.520	31.498	56.383	1.00	54.22	6
N.T		ATOM	961	CG	ARG			31.267	30.012	56.059	1.00	64.20	6
luk.	30	ATOM	962	CD	ARG	Α	391	29.930	29.489	56.602	1.00	73.80	6
14		ATOM	963	NE	ARG	Α	391	29.787	28.044	56.454	1.00	79.76	7
11		ATOM	964	CZ	ARG	Α	391	30.573	27.140	57.043	1.00	84.27	6
in.		ATOM	965		ARG			31.598	27.535	57.806	1.00	85.28	7
W		ATOM	966		ARG			30.340	25.840	56.849	1.00	86.84	7
	35	ATOM	967	С	ARG	Α	391	32.922	31.986	54.358	1.00	48.18	6
1		ATOM	968	0	ARG	Α	391	33.494	31.080	53.756	1.00	49.57	8
11		ATOM	969	N	ILE	Α	392	32.281	32.993	53.762	1.00	45.01	7
C		ATOM	970	CA	ILE	Α	392	32.196	33.148	52.319	1.00	48.77	6
		ATOM	971	CB	ILE	Α	392	31.224	34.297	51.963	1.00	46.45	6
	40	ATOM	972	CG2	ILE	Α	392	31.241	34.582	50.479	1.00	42.35	6
		ATOM	973	CG1	ILE	Α	392	29.791	33.953	52.402	1.00	49.69	6
		ATOM	974	CD1	ILE	Α	392	28.792	35.039	52.113	1.00	51.09	6
		ATOM	975	С	ILE	Α	392	33.554	33.356	51.641	1.00	50.90	6
		ATOM	976	0	ILE	Α	392	33.914	32.605	50.732	1.00	52.21	8
	45	ATOM	977	N	GLU	Α	393	34.298	34.374	52.071	1.00	50.43	7
		ATOM	978	CA	GLU	Α	393	35.592	34.684	51.471	1.00	50.30	6
		ATOM	979	CB	GLU	Α	393	36.437	35.561	52.387	1.00	53.97	6
		ATOM	980	CG	GLU	Α	393	36.558	36.966	51.844	1.00	62.18	6
		ATOM	981	CD	GLU	Α	393	37.546	37.777	52.564	1.00	67.69	6
	50	ATOM	982	OE1	GLU	Α	393	38.149	38.741	52.119	1.00	66.42	8
		ATOM	983	OE2	GLU	Α	393	37.856	37.640	53.729	1.00	70.64	8
		ATOM	984	С	GLU	Α	393	36.341	33.429	51.230	1.00	49.31	6
		ATOM	985	0	GLU	Α	393	36.755	33.089	50.125	1.00	49.53	8
		ATOM	986	N			394	36.552	32.730	52.303	1.00	46.07	7
	55	ATOM	987	CA			394	37.265	31.543	52.078	1.00	45.76	6
		ATOM	988	CB	LYS	Α	394	37.396	30.800	53.373	1.00	43.85	6
		ATOM	989	CG	LYS	Α	394	38.207	31.617	54.394	1.00	40.00	6
		ATOM	990	CD			394	39.372	32.374	53.705	1.00	40.00	6

	5	ATOM	1045	CD1	LEU	Α	400	39.803	34.531	44.256	1.00	26.60	6
		ATOM	1046	CD2	LEU	Α	400	39.065	33.479	42.137	1.00	29.44	6
		ATOM	1047	С	LEU	Α	400	40.941	29.872	42.947	1.00	38.84	6
		ATOM	1048	0	LEU	А	400	41.367	29.632	41.821	1.00	40.38	8
		ATOM	1049	N	LEU			41.464	29.350	44.055	1.00	42.79	7
	10	ATOM	1050	CA	LEU			42.605	28.449	43.988		43.48	6
	10	ATOM	1051	CB	LEU			42.900	27.821	45.355		44.73	6
			1051	CG	LEU			44.105	26.899	45.354		51.39	6
		ATOM						45.374	27.749	45.143		50.11	6
		ATOM	1053		LEU			44.205	26.122	46.662		49.30	6
		ATOM	1054		LEU							41.62	6
	15	ATOM	1055	С	LEU			42.324	27.340	42.981			8
		ATOM	1056	0	LEU			43.052	27.180	42.004		45.14	7
		ATOM	1057	N	ALA			41.269	26.574	43.245		37.92	
		ATOM	1058	CA	ALA			40.873	25.469	42.386		29.90	6
		ATOM	1059	CB	ALA			39.522	24.928	42.834		30.70	6
	20	ATOM	1060	C	ALA			40.798	25.909	40.929		28.88	6
		ATOM	1061	0	ALA	Α	402	41.277	25.203	40.034		32.14	8
		ATOM	1062	N	PHE	Α	403	40.200	27.086	40.707		31.07	7
		MOTA	1063	CA	PHE	Α	403	40.052	27.642	39.363		29.90	6
144		MOTA	1064	CB	PHE	Α	403	39.379	29.019	39.438		27.03	6
1/3	25	ATOM	1065	CG	PHE	Α	403	38.943	29.574	38.100	1.00	26.97	6
11,1		ATOM	1066	CD1	PHE	Α	403	38.228	30.758	38.033	1.00	25.55	6
177		ATOM	1067	CD2	PHE	Α	403	39.224	28.905	36.925	1.00	19.75	6
eri-		ATOM	1068	CE1	PHE	Α	403	37.784	31.266	36.808	1.00	27.90	6
24		ATOM	1069	CE2	PHE	Α	403	38.780	29.416	35.694	1.00	22.56	6
god.	30	ATOM	1070	CZ	PHE	А	403	38.063	30.596	35.640	1.00	22.24	6
14		ATOM	1071	С	PHE	Α	403	41.429	27.756	38.719	1.00	28.82	6
51		MOTA	1072	0	PHE			41.666	27.210	37.646	1.00	26.00	8
13		ATOM	1073	N	GLU	Α	404	42.329	28.463	39.402	1.00	30.25	7
1.4		ATOM	1074	CA	GLU	Α	404	43.695	28.665	38.922	1.00	34.03	6
11	35	ATOM	1075	CB	GLU	А	404	44.513	29.416	39.983	1.00	39.45	6
1.2		ATOM	1076	CG	GLU	Α	404	45.867	29.935	39.489	1.00	47.68	6
.0		ATOM	1077	CD	GLU	А	404	46.734	30.507	40.571	1.00	54.02	6
1		ATOM	1078	OE1	GLU	А	404	46.236	31.298	41.408	1.00	57.27	8
		ATOM	1079		GLU			47.956	30.202	40.606	1.00	63.85	8
	40	ATOM	1080	C	GLU			44.352	27.322	38.634	1.00	36.01	6
		ATOM	1081	ō	GLU			44.936	27.112	37.574	1.00	38.64	8
		ATOM	1082	N	HIS			44.259	26.420	39.610		29.56	7
		ATOM	1083	CA	HIS		405	44.840	25.093	39.468	1.00	31.69	6
		ATOM	1084	CB			405	44.540	24.228	40.694		33.75	6
	45	ATOM	1084	CG	HIS			45.292	24.657	41.908		34.75	6
	43				HIS			46.198	25.640	42.130		34.58	6
		ATOM	1086		HIS			45.161	23.984	43.130		32.43	7
		ATOM	1087					45.975	24.568	44.018		36.15	6
		ATOM	1088		HIS				25.561	43.430		39.84	7
		ATOM	1089		HIS			46.601		38.225		34.21	6
	50	ATOM	1090	С			405	44.274	24.445			37.06	8
		ATOM	1091	0			405	45.029	23.949	37.386			7
		ATOM	1092	N			406	42.947	24.453	38.100		30.83	
		ATOM	1093	CA			406	42.313	23.859	36.930		28.85	6
		ATOM	1094	CB			406	40.805	24.080	36.934		31.48	6
	55	ATOM	1095	CG			406	40.139	23.494	35.709		23.49	6
		ATOM	1096	CD1			406	40.073	22.123	35.532		19.42	6
		ATOM	1097	CE1			406	39.517	21.577	34.382		23.80	6
		ATOM	1098	CD2	TYR	A	406	39.646	24.313	34.704	1.00	21.81	6

	5	ATOM	1099	CE2	TYR .	Α	406	39.090	23.769	33.551	1.00	24.64	6
		ATOM	1100	CZ	TYR .	Α	406	39.029	22.395	33.380	1.00	21.56	6
		ATOM	1101	OH	TYR .	A	406	38.489	21.850	32.236	1.00	24.96	8
		ATOM	1102	С	TYR .	Α	406	42.882	24.504	35.672	1.00	24.24	6
		ATOM	1103	0	TYR .	A	406	42.958	23.872	34.621	1.00	27.08	8
	10	MOTA	1104	N	ILE .	Α	407	43.253	25.784	35.807	1.00	25.76	7
		ATOM	1105	CA	ILE .	Α	407	43.824	26.548	34.705	1.00	33.75	6
		ATOM	1106	CB	ILE .	Α	407	43.986	28.033	35.070	1.00	34.23	6
		ATOM	1107	CG2	ILE .	Α	407	44.967	28.712	34.139	1.00	32.46	6
		ATOM	1108	CG1	ILE .	Α	407	42.615	28.728	35.042	1.00	43.30	6
	15	ATOM	1109	CD1	ILE .	Α	407	41.896	28.602	33.694	1.00	40.40	6
		ATOM	1110	С	ILE .	А	407	45.143	25.973	34.256	1.00	39.03	6
		ATOM	1111	0	ILE .	Α	407	45.383	25.771	33.063	1.00	35.18	8
		ATOM	1112	N	ASN .	A	408	46.003	25.721	35.227	1.00	37.25	7
		MOTA	1113	CA	ASN .		408	47.307	25.194	34.926	1.00	37.01	6
	20	MOTA	1114	CB	ASN .		408	48.107	25.017	36.213	1.00	32.27	6
		ATOM	1115	CG	ASN .	Α	408	48.346	26.362	36.936	1.00	33.56	6
		ATOM	1116	OD1	ASN .	Α	408	48.827	27.335	36.320	1.00	31.99	8
		MOTA	1117	ND2	ASN .	Α	408	48.038	26.403	38.231	1.00	31.23	7
(10)		ATOM	1118	С	ASN.	Α	408	47.205	23.892	34.136	1.00	38.14	6
1D	25	ATOM	1119	0	ASN	Α	408	47.900	23.734	33.124	1.00	42.16	8
IU		ATOM	1120	N	TYR	Α	409	46.334	22.981	34.568	1.00	35.62	7
10		ATOM	1121	CA	TYR	A	409	46.159	21.710	33.866	1.00	35.91	6
j.di		ATOM	1122	CB	TYR	Α	409	45.051	20.859	34.507	1.00	34.41	6
100		ATOM	1123	CG	TYR	А	409	44.624	19.687	33.619	1.00	38.73	6
20031	30	ATOM	1124	CD1	TYR	Α	409	45.563	18.765	33.155	1.00	41.34	6
14		ATOM	1125	CE1	TYR	Α	409	45.186	17.709	32.321	1.00	47.16	6
8)		MOTA	1126	CD2	TYR	Α	409	43.292	19.515	33.232	1.00	46.20	6
(m)		MOTA	1127	CE2	TYR	Α	409	42.913	18.455	32.397	1.00	50.74	6
Į.J		MOTA	1128	CZ	TYR	Α	409	43.863	17.551	31.946	1.00	50.88	6
	35	ATOM	1129	OH	TYR	Α	409	43.498	16.514	31.130	1.00	53.14	8
100		MOTA	1130	C	TYR	Α	409	45.760	21.966	32.424		38.16	6
*D		ATOM	1131	0	TYR	Α	409	46.202	21.281	31.502		41.83	8
722		MOTA	1132	N	ARG	Α	410	44.872	22.943	32.272		42.25	7
		ATOM	1133	CA	ARG	Α	410	44.345	23.332	30.984		42.83	6
	40	MOTA	1134	CB	ARG	Α	410	43.311	24.427	31.195		36.83	6
		ATOM	1135	CG	ARG	Α	410	41.994	23.979	31.795		34.32	6
		ATOM	1136	CD	ARG			41.073	23.504	30.675		36.62	6
		ATOM	1137	NE	ARG			40.888	24.550	29.685		38.64	7
		ATOM	1138	CZ	ARG			40.177	24.397	28.576		35.73	6
	45	ATOM	1139		ARG			39.572	23.230	28.348		33.17	7
		ATOM	1140		ARG			40.077	25.407	27.708		32.70	7
		ATOM	1141	С	ARG			45.442	23.850	30.083		46.67	6
		ATOM	1142	0	ARG			45.467	23.591	28.882		41.78	8
		MOTA	1143	N	LYS			46.360	24.577	30.710		52.99	7
	50	MOTA	1144	CA	LYS			47.467	25.194	30.017		58.32	6
		ATOM	1145	CB	LYS			48.645	24.216	29.876		64.99	6
		ATOM	1146	ÇG	LYS			48.349	22.835	29.367		70.48	6
		MOTA	1147	CD	LYS			49.608	21.974	29.494		77.18	6
		MOTA	1148	CE	LYS			49.461	20.621	28.795		84.30	6
	55	ATOM	1149	NZ	LYS			50.740	19.828	28.857		86.48	7
		ATOM	1150	С	LYS			47.032	25.756	28.686		56.66	6
		ATOM	1151	0	LYS			47.160	25.153	27.633		55.47	8
		ATOM	1152	N	HIS	А	412	46.458	26.943	28.823	1.00	54.67	7

	5	20014	1061		T 1/0	70	404	38.79	11 20	.752	33.975	1 00	31.56	7
	3	ATOM	1261	N	LYS									
		ATOM	1262	CA	LYS			37.47		.529	33.423		32.29	6
		ATOM	1263	CB	LYS	А	424	37.44	16 38	.205	32.658		30.56	6
		ATOM	1264	CG	LYS	Α	424	38.39	94 38	.192	31.455	1.00	30.07	6
		ATOM	1265	CD	LYS	Α	424	38.05	50 39	.326	30.488	1.00	33.22	6
	10	ATOM	1266	CE	LYS			39.03	32 39	.433	29.322	1.00	28.75	6
		ATOM	1267	NZ	LYS			40.39	94 39	.942	29.707	1.00	31.01	7
		ATOM	1268	C	LYS			36.4		.558	34.524		29.26	6
		ATOM	1269	0	LYS			35.30		.998	34.289		30.22	8
					VAL			36.79		.098	35.719		23.53	7
		ATOM	1270	N							36.866		28.91	6
	15	ATOM	1271	CA	VAL		425	35.89		.107				
		ATOM	1272	CB	VAL			36.5		.460	38.094		29.44	6
		ATOM	1273		VAL			35.6		.642	39.320		28.81	6
		ATOM	1274	CG2	VAL			36.7		.985	37.849		31.22	6
		ATOM	1275	С	VAL	Α	425	35.5	12 40	.548	37.161		32.03	6
	20	ATOM	1276	0	VAL	Α	425	34.3	50 40	.839	37.429	1.00	31.95	8
		ATOM	1277	N	THR	Α	426	36.49	96 41	.444	37.124	1.00	33.61	7
		ATOM	1278	CA	THR	Α	426	36.2	48 42	.866	37.356	1.00	30.76	6
		ATOM	1279	CB	THR			37.5	59 43	670	37.360	1.00	32.34	6
200	ne.	ATOM	1280		THR			38.20		3.565	38.630	1.00	33.07	8
10	5 25	ATOM	1281		THR			37.30		.131	37.015	1.00	25.40	6
15	11	ATOM	1282	C	THR			35.3		3.324	36.211		32.53	6
Ü	n	ATOM	1283	Ö	THR			34.3		1.006	36.405		35.19	8
5					ASP			35.7		2.929	35.006		28.83	7
3		ATOM	1284	N	ASP			35.0		3.272	33.810		35.12	6
		ATOM	1285	CA									39.14	6
1	30	MOTA	1286	CB	ASP			35.5		2.524	32.578			6
11		ATOM	1287	CG	ASP		427	36.8		3.103	32.057		45.80	
41.00		ATOM	1288		ASP			36.9		1.346	32.024		41.97	8
1	· 1	ATOM	1289		ASP			37.7		2.333	31.616		50.06	8
1	는 - 1	ATOM	1290	С	ASP			33.5		2.925	34.028		33.94	6
1,	35	ATOM	1291	0	ASP			32.6		3.712	33.702		38.02	8
1	ad No	ATOM	1292	N	LEU	А	428	33.2		.745	34.584		27.15	7
		ATOM	1293	CA	LEU	Α	428	31.9	25 41	1.293	34.850		29.99	6
1	U	ATOM	1294	CB	LEU	Α	428	31.9	24 39	786	35.133	1.00	22.49	6
		ATOM	1295	CG	LEU	Α	428	32.1	04 38	3.873	33.939	1.00	25.54	6
	40	ATOM	1296	CD1	LEU	Α	428	32.2	02 37	7.421	34.353	1.00	20.60	6
		ATOM	1297	CD2	LEU	Α	428	30.9	20 39	0.083	33.029	1.00	17.24	6
		ATOM	1298	С			428	31.2	76 42	2.057	35.991	1.00	28.94	6
		ATOM	1299	0	LEU			30.0		2.306	35.939	1.00	31.26	8
		ATOM	1300	N			429	32.0		2.423	37.011	1.00	27.64	7
	45	ATOM	1301	CA			429	31.5		3.162	38.147	1.00	28.13	6
	15	ATOM	1302	CB			429	32.5		3.298	39.264		29.59	6
		ATOM	1302	CG			429	32.8		2.040	40.080		34.85	6
							429	33.5		2.360	41.367		47.18	6
		ATOM	1304	CD				34.0		1.175	42.049		57.93	7
	~~	ATOM	1305	NE			429				42.547		63.62	6
	50	ATOM	1306	CZ			429	33.3).210				7
		ATOM	1307		ARG			31.9		270	42.396		60.71	
		ATOM	1308		ARG			33.9		.165	43.150		62.38	7
		ATOM	1309	C			429	31.0		1.536	37.707		29.81	6
		ATOM	1310	0			429	30.0		5.009	38.101		30.81	8
	55	ATOM	1311	N	MET	Α	430	31.9		5.176	36.901		29.64	7
		ATOM	1312	CA	MET	Α	430	31.6		5.502	36.383		34.72	6
		ATOM	1313	CB	MET	Α	430	32.7	45 46	5.955	35.434	1.00	34.97	6
		ATOM	1314	CG	MET	Α	430	33.9	37 47	7.597	36.080	1.00	45.34	6

	_					_		00 500	40 100	26 022	1 00	52.55	16
	5	ATOM	1315	SD	MET			33.520	49.120	36.937			
		ATOM	1316	CE	MET			32.942	50.174	35.585		55.56	6
		MOTA	1317	С	MET			30.315	46.455	35.634		34.01	6
		ATOM	1318	0	MET	Α	430	29.455	47.295	35.854		37.29	8
		ATOM	1319	N	ILE	Α	431	30.180	45.468	34.740		29.99	7
	10	ATOM	1320	CA	ILE	Α	431	28.954	45.269	33.969	1.00	28.82	6
		ATOM	1321	CB	ILE	Α	431	28.962	43.936	33.211	1.00	27.39	6
		ATOM	1322	CG2	ILE	Α	431	27.622	43.671	32.572	1.00	23.87	6
		ATOM	1323	CG1	ILE			30.044	43.920	32.138	1.00	25.56	6
		ATOM	1324		ILE			29.989	42.703	31.244	1.00	17.29	6
	15	ATOM	1325	C	ILE			27.769	45.269	34.907		29.49	6
	13			0	ILE			26.810	45.993	34.712		24.19	8
		ATOM	1326	N	GLY			27.839	44.435	35.936		25.25	7
		ATOM	1327		GLY			26.748	44.343	36.890		30.38	6
		ATOM	1328	CA				26.494	45.671	37.554		32.75	6
		ATOM	1329	C	GLY					37.469		36.38	8
	20	MOTA	1330	0	GLY			25.411	46.206				7
		MOTA	1331	N	ALA			27.514	46.189	38.221		26.77	
		ATOM	1332	CA	ALA			27.428	47.459	38.910		26.48	6
		ATOM	1333	CB	ALA			28.836	47.970	39.203		19.90	6
(7)		ATOM	1334	С	ALA			26.663	48.502	38.114		30.73	6
+0	25	MOTA	1335	0	ALA			25.773	49.164	38.635		31.60	8
1		ATOM	1336	N	CYS			27.027	48.654	36.854		33.22	7
(2)		ATOM	1337	CA	CYS	А	434	26.371	49.616	35.996		34.34	6
goods.		ATOM	1338	CB	CYS	А	434	27.047	49.612	34.711		35.20	6
1		ATOM	1339	SG	CYS	Α	434	27.789	50.811	34.285		54.48	16
india.	30	ATOM	1340	С	CYS	Α	434	24.974	49.198	35.612		34.09	6
		ATOM	1341	0	CYS	Α	434	24.107	50.040	35.415		34.89	8
21 ages.		ATOM	1342	N	HIS	Α	435	24.756	47.898	35.447		34.30	7
Lat.		ATOM	1343	CA	HIS	Α	435	23.453	47.423	35.042		35.44	6
Li]		ATOM	1344	CB	HIS	Α	435	23.404	45.904	35.104	1.00	31.76	6
1,1	35	ATOM	1345	CG	HIS	Α	435	22.099	45.351	34.675	1.00	32.03	6
Tue!		ATOM	1346	CD2	HIS	Α	435	21.697	44.790	33.519	1.00	28.61	6
0		ATOM	1347	ND1	HIS	Α	435	20.941	45.482	35.452	1.00	28.48	7
Ü		ATOM	1348	CE1	HIS	Α	435	19.912	45.025	34.759	1.00	33.27	6
		ATOM	1349		HIS			20.345	44.597	33.583	1.00	31.57	7
	40	ATOM	1350	С			435	22.400	47.974	35.972	1.00	32.74	6
		ATOM	1351	0			435	21.304	48.284	35.565	1.00	32.87	8
		ATOM	1352	N			436	22.777	48.046	37.241	1.00	31.01	7
		ATOM	1353	CA			436	21.910	48.563	38.266	1.00	29.91	6
		ATOM	1354	CB			436	22.661	48.595	39.580	1.00	21.23	6
	45		1355	C			436	21.475	49.969	37.884		33.86	6
	43	ATOM		0			436	20.296	50.298	37.910		36.10	8
		ATOM	1356					22.453	50.795	37.532		35.19	7
		ATOM	1357	N			437	22.172	52.167	37.140		33.03	6
		ATOM	1358	CA			437		52.815	36.603		35.31	6
		ATOM	1359	CB			437	23.441		36.193		44.99	8
	50	ATOM	1360	OG			437	23.203	54.151			38.39	6
		ATOM	1361	С			437	21.110	52.158	36.055			
		ATOM	1362	0			437	20.049	52.745	36.204		37.54	8
		ATOM	1363	N			438	21.432	51.483	34.956		37.32	7
		ATOM	1364	CA			438	20.534	51.379	33.821		39.30	6
	55	ATOM	1365	CB			438	21.114	50.402	32.786		42.97	6
		ATOM	1366	CG			438	22.343	50.911	32.051		41.72	6
		ATOM	1367	CD			438	21.955	52.134	31.251		45.23	6
		ATOM	1368	NE	ARG	Α	438	20.964	51.839	30.237	1.00	45.66	7

	5	ATOM	1369	CZ	ARG	Α	438	20.063	52.718	29.809	1.00	49.71	6
		ATOM	1370	NH1	ARG	Α	438	20.046	53.958	30.318	1.00	50.91	7
		ATOM	1371	NH2	ARG	Α	438	19.198	52.354	28.865	1.00	46.86	7
		ATOM	1372	С	ARG	А	438	19.147	50.922	34.240	1.00	42.37	6
		ATOM	1373	0	ARG			18.147	51.297	33.625	1.00	40.58	8
	10	ATOM	1374	N	PHE			19.080	50.120	35.298		42.25	7
		ATOM	1375	CA	PHE			17.803	49.624	35.763	1.00	42.81	6
		ATOM	1376	CB	PHE			17.975	48.794	37.013	1.00	42.18	6
		ATOM	1377	CG	PHE			16.739	48.053	37.413	1.00	42.48	6
		ATOM	1378		PHE			16.198	47.111	36.562		47.09	6
	15	ATOM	1379	CD2	PHE			16.105	48.320	38.613		39.76	6
	13	ATOM	1380	CE1	PHE			15.047	46.427	36.905		49.17	6
		ATOM	1381	CE2	PHE			14.940	47.630	38.963		45.10	6
		ATOM	1382	CZ	PHE			14.411	46.683	38.098		46.36	6
		ATOM	1383	C	PHE			16.921	50.803	36.075		44.79	6
	20	ATOM	1384	0	PHE			15.830	50.903	35.554		40.26	8
	20	ATOM	1385	N	LEU			17.410	51.681	36.951		42.77	7
			1386	CA	LEU			16.660	52.871	37.344		42.96	6
		ATOM	1387	CB	LEU			17.546	53.824	38.150		37.19	6
, cts		ATOM		CG	LEU			17.943	53.297	39.500		36.97	6
40	25	ATOM	1388 1389		LEU			18.620	54.389	40.316		33.65	6
150	23	ATOM			LEU			16.679	52.837	40.216		35.42	6
10		ATOM	1390	CD2				16.025	53.596	36.168		45.47	6
Sect.		ATOM	1391		LEU			14.809	53.750	36.126		52.48	8
S		ATOM	1392	0	LEU			16.836	54.060	35.223		49.15	7
j.s.	30	ATOM	1393 1394	N	HIS			16.277	54.725	34.063		54.76	6
300	30	ATOM	1394	CA CB	HIS		441	17.329	54.955	33.031		56.68	6
85		MOTA	1396	CG	HIS			18.134	56.161	33.282		62.73	6
100		ATOM			HIS			18.468	57.216	32.499		65.73	6
111		ATOM	1397		HIS			18.701	56.431	34.538		66.01	7
1.J	25	ATOM	1398					19.332	57.594	34.473		65.55	6
	35	ATOM	1399		HIS			19.332	58.085	33.255		60.09	7
1		ATOM	1400		HIS			15.244	53.822	33.481		55.93	6
20		ATOM	1401	C				14.149	54.263	33.170		57.33	8
		ATOM	1402 1403	O N	HIS			15.605	52.549	33.313		57.81	7
	40	ATOM	1403	CA	MET			14.661	51.583	32.778		59.11	6
	40	MOTA	1404	CB	MET			15.191	50.154	32.922		55.93	6
		MOTA	1405	CG	MET			16.336	49.813	32.022		58.52	6
		MOTA		SD	MET			16.681	48.008	31.851		60.99	16
		MOTA	1407 1408	CE	MET			17.085	47.602	33.581		52.61	6
	15	ATOM		CE	MET			13.339	51.727	33.534		60.31	6
	45	MOTA	1409		MET			12.266	51.560	32.968		58.18	8
		ATOM	1410	0	LYS			13.425	52.054	34.818		61.45	7
		ATOM	1411	N	LYS			12.236	52.202	35.626		64.90	6
		ATOM	1412	CA			443	12.236	52.202	37.020		64.40	6
	50	ATOM	1413	CB					51.748	37.959		69.12	6
	50	MOTA	1414	CG	LYS			11.461 12.068	51.551	39.257		71.14	6
		MOTA	1415	CD	LYS					40.091		73.43	6
		MOTA	1416	CE			443	11.368	51.897			67.97	7
		ATOM	1417	NZ	LYS			11.883	51.712	41.415 35.348		67.29	6
		ATOM	1418	С			443	11.513	53.514 53.700	35.780		67.90	8
	55	MOTA	1419	0			443	10.390 12.171	54.429	34.629		66.57	7
		ATOM	1420	N	VAL				55.719	34.297		64.76	6
		MOTA	1421	CA	VAL			11.575		34.297		62.76	6
		MOTA	1422	CB	VAL	А	444	12.569	56.869	54.500	1.00	02.70	0

	5	ATOM	1423	CC1	VAL	n	111	11.952	58.195	34.174	1.00	64.00	6
	,	ATOM	1424		VAL			12.999	56.891	36.035		59.27	6
				C	VAL			11.043	55.730	32.861		68.61	6
		ATOM	1425					9.937	56.210	32.612		70.60	8
		ATOM	1426	0	VAL				55.173	31.935		70.71	7
		ATOM	1427	N	GLU			11.814	55.152	30.514		71.45	6
	10	ATOM	1428	CA	GLU			11.457				72.36	6
		ATOM	1429	CB	GLU		445	12.725	55.255	29.664			6
		ATOM	1430	CG	GLU			13.598	56.429	30.022		40.00	
		ATOM	1431	CD	GLU			14.875	56.472	29.239		40.00	6
		ATOM	1432	OE1	GLU			15.155	55.565	28.414		40.00	8
	15	ATOM	1433	OE2	GLU			15.663	57.430	29.430		40.00	8
		ATOM	1434	С	GLU			10.724	53.912	30.049		71.46	6
		ATOM	1435	0	GLU	Α	445	10.536	53.701	28.844		73.02	8
		ATOM	1436	N	CYS	Α	446	10.301	53.099	30.999		71.12	7
		ATOM	1437	CA	CYS	Α	446	9.628	51.899	30.634		70.83	6
	20	ATOM	1438	CB	CYS	Α	446	10.595	50.719	30.687		71.05	6
		ATOM	1439	SG	CYS	Α	446	12.009	50.842	29.573		72.83	16
		ATOM	1440	С	CYS	Α	446	8.454	51.671	31.535	1.00	71.91	6
		ATOM	1441	0	CYS	Α	446	8.495	52.014	32.728	1.00	72.06	8
(2)		ATOM	1442	N	PRO	Α	447	7.372	51.133	30.978	1.00	73.12	7
40	25	ATOM	1443	CD	PRO	Α	447	7.267	50.764	29.560	1.00	72.88	6
14		ATOM	1444	CA	PRO	Α	447	6.150	50.853	31.740	1.00	74.22	6
(0)		ATOM	1445	CB	PRO	Α	447	5.187	50.281	30.714	1.00	72.98	6
2:2		ATOM	1446	CG	PRO			5.875	50.271	29.437	1.00	74.77	6
14		ATOM	1447	С	PRO			6.435	49.843	32.831	1.00	75.94	6
peres.	30	ATOM	1448	ō	PRO			7.181	48.908	32.612	1.00	76.67	8
16		ATOM	1449	N	THR		448	5.820	50.002	33.997	1.00	76.91	7
0		ATOM	1450	CA	THR			6.024	49.066	35.113	1.00	78.24	6
\$100 B		ATOM	1451	CB	THR			5.528	49.734	36.401	1.00	81.33	6
LL		ATOM	1452		THR			4.105	49.917	36.328	1.00	84.46	8
	35	ATOM	1453		THR			6.192	51.081	36.585	1.00	83.51	6
1,2	-	ATOM	1454	С	THR			5.113	47.912	34.755	1.00	77.42	6
·D		ATOM	1455	ō	THR			4.915	46.995	35.519	1.00	77.65	8
18)		ATOM	1456	N	GLU			4.539	48.021	33.565	1.00	76.29	7
		ATOM	1457	CA	GLU			3.630	47.023	33.024	1.00	75.03	6
	40	ATOM	1458	СВ	GLU			2.600	47.773	32.191	1.00	74.62	6
	-10	ATOM	1459	CG	GLU			2.145	47.051	31.001	1.00	40.00	6
		ATOM	1460	CD	GLU			1.297	47.889	30.178	1.00	40.00	6
		ATOM	1461		GLU			1.479	49.137	30.146	1.00	40.00	8
		ATOM	1462		GLU			0.424	47.322	29.497	1.00	40.00	8
	45	ATOM	1463	C	GLU			4.434	46.036	32.179		73.49	6
	13	ATOM	1464	Ö	GLU			3.882	45.142	31.559	1.00	70.24	8
		ATOM	1465	И	LEU			5.747	46.224	32.161		70.80	7
		ATOM	1466	CA	LEU			6.608	45.347	31.378	1.00	68.82	6
		ATOM	1467	CB	LEU			7.301	46.154	30.277		71.91	6
	50	ATOM	1468	CG			450	6.464	46.819	29.217		76.62	6
	30				LEU			7.337	47.662	28.328		77.95	6
		ATOM	1469					5.786	45.750	28.415		76.46	6
		ATOM	1470		LEU			7.669	44.673	32.243		66.22	6
		ATOM	1471	С			450		43.841	31.752		66.01	8
		ATOM	1472	0			450	8.427 7.705	45.039	33.530		61.96	7
	55	ATOM	1473	N			451	8.681	44.506	34.480		58.44	6
		ATOM	1474	CA			451	9.041	45.562	35.540		61.34	6
		ATOM	1475	CB			451					63.02	6
		MOTA	1476	CG	PHE	Α	451	9.873	46.717	35.008	1.00	03.02	0

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	5	ATOM	1531	CD	GLU	Α	457	10.807	37.994	44.648	1.00	20.00	6
		ATOM	1532	OE1	GLU	Α	457	11.673	37.099	44.311	1.00	20.00	8
			1533	OE2	GLU			9.683	37.639	45.172	1 00	20.00	8
		ATOM										43.21	7
		ATOM	1534	И	VAL			14.928	41.078	41.903			
		ATOM	1535	CA	VAL	Α	458	16.412	41.094	41.868		44.98	6
	10	ATOM	1536	CB	VAL	Α	458	16.881	40.306	40.642	1.00	44.83	6
		ATOM	1537	CGI	VAL	Δ	458	18.365	40.106	40.698	1.00	49.72	6
								16.185	38.979	40.558		40.89	6
		ATOM	1538		VAL								
		ATOM	1539	C	VAL			17.130	42.420	41.877		42.72	6
		ATOM	1540	0	VAL	Α	458	18.061	42.617	42.658	1.00	42.88	8
	15	ATOM	1541	N	PHE	Α	459	16.713	43.325	41.010	1.00	44.53	7
		ATOM	1542	CA	PHE	Δ	459	17.385	44.606	40.892	1.00	48.18	6
			1543	CB	PHE			17.281	45.104	39.494		43.60	6
		ATOM											6
		ATOM	1544	CG	PHE			17.915	44.190	38.547		40.79	
		ATOM	1545	CD1	PHE	Α	459	17.325	42.983	38.244		41.01	6
	20	ATOM	1546	CD2	PHE	Α	459	19.153	44.483	38.054	1.00	39.48	6
		ATOM	1547	CE1	PHE	А	459	17.988	42.081	37.441	1.00	40.62	6
		ATOM	1548		PHE			19.814	43.589	37.257	1.00	36.87	6
					PHE			19.233	42.385	36.940		36.39	6
		ATOM	1549	CZ									
100		ATOM	1550	С	PHE	Α	459	16.837	45.648	41.744		52.71	6
10	25	ATOM	1551	0	PHE	Α	459	17.492	46.682	42.017		51.34	8
173		ATOM	1552	N	GLU	Α	460	15.606	45.422	42.161	1.00	62.92	7
170		ATOM	1553	CA	GLU			15.066	46.428	42.965	1.00	69.33	6
find.		ATOM	1554	CB	GLU			13.552	46.352	43.094	1 00	72.95	6
10.5									47.767	42.957		78.35	6
		MOTA	1555	CG	GLU			12.978					
jedi.	30	ATOM	1556	CD	GLU			12.246	48.261	44.157		82.97	6
14		ATOM	1557	OE1	GLU	Α	460	12.471	47.759	45.281	1.00	88.28	8
20		ATOM	1558	OE2	GLU	Α	460	11.422	49.200	44.017	1.00	84.80	8
13		ATOM	1559	С	GLU	Α	460	15.736	46.245	44.272	1.00	71.87	6
12			1560	o	GLU			16.187	45.170	44.691	1.00	74.51	8
	2.5	ATOM								44.917		78.50	7
gran.	35	MOTA	1561	N	ASP			15.790	47.373				
1153		ATOM	1562	CA	ASP			16.415	47.505	46.173		84.19	6
10		MOTA	1563	CB	ASP	Α	461	16.394	48.981	46.471	1.00	85.82	6
13.5		ATOM	1564	CG	ASP	Α	461	16.801	49.786	45.276	1.00	89.62	6
		ATOM	1565	OD1	ASP			16.692	49.344	44.086	1.00	93.00	8
	40		1566		ASP			17.239	50.923	45.482	1.00	93.04	8
	40	ATOM						15.639	46.703	47.214		86.80	6
		ATOM	1567	С	ASP								8
		ATOM	1568	0			461	16.245	45.748	47.731		88.70	
		ATOM	1569	OXT	ASP	Α	461	14.457	47.026	47.451	1.00	88.70	8
		TER											
	45	ATOM	1	CB	T.YS	R	211	-20.802	66.251	39.780	1.00	46.72	6
	15	ATOM	2	CG			211	-19.566	65.345	39.922	1.00	56.48	6
										40.045		60.93	6
		MOTA	3	CD			211	-18.264	66.114				
		ATOM	4	CE	LYS	В	211	-18.043	67.067	38.886		61.95	6
		ATOM	5	NZ	LYS	В	211	-19.008	68.224	38.903	1.00	69.93	7
	50	ATOM	6	С	LYS	В	211	-22.418	67.861	40.818	1.00	35.68	6
		ATOM	7	0			211	-23.356	67.113	40.454	1.00	33.58	8
			8				211	-20.742	66.675	42.239	1 00	45.76	7
		MOTA		N									
		ATOM	9	CA			211	-20.998	67.285	40.894		43.42	6
		MOTA	10	N	PRO	В	212	-22.610	69.205	41.068		35.64	7
	55	ATOM	11	CD	PRO	В	212	-21.526	70.177	41.287	1.00	38.60	6
		ATOM	12	CA			212	-23.943	69.861	41.036	1.00	38.35	6
		ATOM	13	CB			212	-23.657	71.320	41.420		38.95	6
										41.551		42.00	6
		MOTA	14	CG	PRO	В	212	-22.226	71.474	41.001	1.00	42.00	0

	5	ATOM	15	С	PRO	В	212	-24.798	69.772	39.807	1.00	38.78	6
		ATOM	16	0	PRO	В	212	-24.350	70.045	38.696	1.00	34.64	8
		ATOM	17	N	GLU	В	213	-26.058	69.424	40.032	1.00	40.31	7
		ATOM	18	CA	GLU	В	213	-27.081	69.290	39.003	1.00	43.87	6
		ATOM	19	CB	GLU	В	213	-27.895	68.004	39.265	1.00	45.16	6
	10	ATOM	20	CG	GLU	В	213	-27.032	66.709	39.286	1.00	47.60	6
		ATOM	21	CD	GLU	В	213	-27.807	65.421	39.199	1.00	50.68	6
		ATOM	22	OE1	GLU	В	213	-28.847	65.244	39.886	1.00	59.18	8
		ATOM	23	OE2	GLU	В	213	-27.382	64.516	38.442	1.00	49.06	8
		ATOM	24	C	GLU	В	213	-27.924	70.576	39.080	1.00	45.96	6
	15	ATOM	25	0	GLU	В	213	-27.624	71.467	39.859	1.00	43.13	8
		ATOM	26	N	PRO	В	214	-28.987	70.698	38.308	1.00	46.52	7
		ATOM	27	CD	PRO	В	214	-29.484	69.635	37.446	1.00	46.44	6
		ATOM	28	CA	PRO	В	214	-29.843	71.907	38.302	1.00	47.52	6
		ATOM	29	CB	PRO	В	214	-30.799	71.639	37.210		45.40	6
	20	MOTA	30	CG	PRO	В	214	-30.530	70.257	36.805		49.89	6
		ATOM	31	С	PRO	В	214	-30.574	72.330	39.535		45.70	6
		ATOM	32	0	PRO	В	214	-30.597	71.595	40.483		44.49	8
		ATOM	33	N	THR	В	215	-31.180	73.515	39.506		45.24	7
(160)		ATOM	34	CA	THR		215	-31.965	74.036	40.652		49.36	6
4Ď	25	ATOM	35	CB	THR			-31.443	75.420	41.091		44.86	6
14		ATOM	36		THR			-32.249	76.464	40.534		52.26	8
(10		ATOM	37		THR		215	-30.011	75.617	40.659		39.43	6
\$100a		ATOM	38	C	THR			-33.386	74.239	40.114		52.51	6
Tools		ATOM	39	0	THR			-33.562	74.868	39.078		53.48	8 7
14	30	ATOM	40	N	ASP			-34.387	73.741	40.829		58.81 61.51	6
10		MOTA	41	CA	ASP			-35.795	73.865	40.435 41.650		70.57	6
Jan 1		ATOM	42	CB	ASP			-36.674	74.005 72.981	41.710		78.07	6
1,1		ATOM	43	CG OD1	ASP ASP			-37.675 -38.228	72.588	40.652		82.31	8
W	35	ATOM	44 45		ASP			-37.983	72.567	42.830		86.55	8
(3)	33	ATOM ATOM	46	C	ASP			-35.920	75.123	39.648		58.42	6
-13		ATOM	47	0	ASP			-36.847	75.317	38.827		56.85	8
ű		ATOM	48	N	GLU			-34.954	75.979	39.984		54.92	7
		ATOM	49	CA	GLU			-34.851	77.259	39.353		53.37	6
	40	ATOM	50	CB			217	-34.104	78.264	40.251	1.00	51.02	6
		ATOM	51	CG			217	-34.151	79.689	39.679	1.00	40.00	6
		ATOM	52	CD			217	-34.301	80.745	40.739	1.00	40.00	6
		ATOM	53		GLU			-34.089	80.443	41.945	1.00	40.00	8
		ATOM	54	OE2				-34.625	81.921	40.411	1.00	40.00	8
	45	ATOM	55	C	GLU	В	217	-34.232	77.163	37.957	1.00	53.55	6
		ATOM	56	0	GLU	В	217	-34.815	77.612	37.018	1.00	54.33	8
		ATOM	57	N	GLU	В	218	-33.063	76.572	37.839		49.20	7
		ATOM	58	CA	GLU	В	218	-32.318	76.385	36.608		45.94	6
		ATOM	59	CB	GLU	В	218	-30.965	75.793	36.981		43.43	6
	50	ATOM	60	CG	GLU	В	218	-30.065	76.728	37.801		40.86	6
		ATOM	61	CD	GLU	В	218	-28.713	76.159	38.072		39.88	6
		ATOM	62	OE1			218	-28.606	74.967	38.449		37.61	8
		ATOM	63	OE2			218	-27.707	76.901	37.945		34.01	8
		ATOM	64	С			218	-33.014	75.475	35.610		44.71	6
	55	MOTA	65	0			218	-32.935	75.686	34.405		45.31	8
		MOTA	66	N			219	-33.669	74.439	36.131		44.02	7
		ATOM	67	CA			219	-34.368	73.490	35.290		46.97	6 6
		MOTA	68	CB	TRP	В	219	-35.046	72.408	36.119	1.00	48.42	О

	5	ATOM	69	CG	TRP	В	219	-34.195	71.230	36.374	1.00	54.61	6
		ATOM	70	CD2	TRP	В	219	-34.048	70.120	35.478	1.00	55.24	6
		ATOM	71	CE2	TRP	В	219	-33.076	69.248	36.063	1.00	53.67	6
		ATOM	72	CE3	TRP	В	219	-34.615	69.771	34.252	1.00	54.55	6
		ATOM	73	CD1	TRP	В	219	-33.399	71.019	37.415	1.00	55.75	6
	10	ATOM	74		TRP		219	-32.697	69.838	37.236	1.00	54.43	7
		ATOM	75		TRP		219	-32.635	68.075	35.431	1.00	52.54	6
		ATOM	76	CZ3	TRP		219	-34.214	68.603	33.643	1.00	55.17	6
		ATOM	77	CH2	TRP		219	-33.234	67.758	34.214	1.00	55.59	6
		ATOM	78	C	TRP		219	-35.409	74.199	34.459		47.32	6
	15	ATOM	79	0	TRP		219	-35.561	73.914	33.277		43.56	8
	13	ATOM	80	N	GLU		220	-36.126	75.130	35.084		49.91	7
		ATOM	81	CA	GLU		220	-37.158	75.874	34.402		53.57	6
		ATOM	82	CB	GLU		220	-37.811	76.820	35.373		58.18	6
		ATOM	83	CG	GLU		220	-39.251	76.812	35.221		73.13	6
	20		84	CD	GLU		220	-39.824	76.858	36.489		80.06	6
	20	ATOM	85	OE1	GLU		220	-39.485	75.995	37.324		82.12	8
		ATOM		OE2	GLU		220	-40.635	77.740	36.718		82.78	8
		ATOM	86		GLU		220	-36.539	76.645	33.250		50.51	6
Visas.		ATOM	87	С			220	-37.160	76.793	32.195		49.94	8
	25	ATOM	88	0	GLU			-35.312	77.135	33.455		43.71	7
0	25	MOTA	89	N	LEU		221		77.884	32.411		42.81	6
10		ATOM	90	CA	LEU		221	-34.604	78.324	32.865		39.21	6
frak		ATOM	91	CB	LEU		221	-33.214 -32.321	78.833	31.754		36.34	6
14		ATOM	92	CG	LEU		221		79.843	30.927		36.93	6
Ente		ATOM	93		LEU			-33.073	79.645	32.331		24.18	6
14,1	30	ATOM	94				221	-31.058	77.011	31.192		43.46	6
31		MOTA	95	С	LEU		221	-34.454		30.104		45.25	8
Parel I		MOTA	96	0	LEU			-34.819	77.406 75.829	31.398		39.09	7
النا		ATOM	97	N	ILE			-33.878				35.47	6
		ATOM	98	CA			222	-33.687	74.857	30.330		33.74	6
u	35	ATOM	99	CB	ILE		222	-33.224	73.516			28.86	6
40		ATOM	100		ILE			-33.204	72.488	29.776		33.33	6
4D		ATOM	101	CG1	ILE			-31.840	73.631	31.493		34.85	6
		ATOM	102	CD1	ILE			-31.435	72.419	32.264		34.26	6
		MOTA	103	С	ILE			-34.991	74.627	29.598			8
	40	ATOM	104	0	ILE			-35.082	74.832	28.392		31.90	7
		ATOM	105	N	LYS			-35.992	74.183	30.346		39.49 44.43	6
		ATOM	106	CA	LYS			-37.300	73.892	29.785			6
		ATOM	107	CB	LYS			-38.351	73.876	30.882		50.81	
	_	ATOM	108	CG	LYS			-39.693	73.358	30.411		62.51	6 6
	45	ATOM	109	CD	LYS			-40.795	73.532	31.449		72.22	
		ATOM	110	CE	LYS			-42.163	73.249	30.827		74.55	6
		ATOM	111	ΝZ	LYS		223	-43.268	73.378	31.837		75.78	7
		ATOM	112	С			223	-37.648	74.942	28.755		42.81	6
		ATOM	113	0			223	-38.337	74.661	27.796		40.36	8
	50	ATOM	114	N	THR		224	-37.146	76.156	28.979		39.89	7
		ATOM	115	CA	THR	В	224	-37.353	77.293	28.074		39.93	6
		ATOM	116	CB	THR		224	-36.956	78.609	28.776		40.57	6
		ATOM	117		THR			-37.646	78.740	30.028		39.27	8
		ATOM	118	CG2	THR			-37.273	79.805	27.893		38.11	6
	55	ATOM	119	С			224	-36.521	77.094	26.789		39.96	6
		ATOM	120	0			224	-37.043	76.677	25.756		36.67	8
		ATOM	121	N	VAL				77.421	26.888		38.02	7
		ATOM	122	CA	VAL	В	225	-34.263	77.295	25.801	1.00	38.12	6

5 ATOM 123 CB VAL B 225 -32.869 77.015 26.348 1.00 38.1 ATOM 124 CG1 VAL B 225 -31.863 76.993 25.266 1.00 36.7 ATOM 125 CG2 VAL B 225 -34.621 76.993 25.266 1.00 36.7 ATOM 127 O VAL B 225 -34.621 76.364 23.638 1.00 37.5 ATOM 127 O VAL B 225 -34.621 76.364 23.638 1.00 36.7 ATOM 128 N THR B 226 -35.005 75.046 25.410 1.00 34.6 ATOM 128 N THR B 226 -35.005 75.046 25.410 1.00 34.6 ATOM 129 CA THR B 226 -35.423 73.887 24.638 1.00 36.7 ATOM 120 CB THR B 226 -35.423 73.887 24.638 1.00 34.6 ATOM 130 CB THR B 226 -35.423 73.887 24.638 1.00 34.6 ATOM 131 OGI THR B 226 -36.643 71.595 24.874 1.00 30.5 ATOM 131 OGI THR B 226 -36.643 71.595 24.874 1.00 20.5 ATOM 132 CG2 THR B 226 -36.643 71.595 24.874 1.00 20.5 ATOM 133 C THR B 226 -36.633 74.054 22.803 1.00 36.4 ATOM 135 N ALA B 227 -37.746 74.542 24.480 1.00 39.2 ATOM 135 N ALA B 227 -37.746 74.542 24.480 1.00 39.2 ATOM 136 CA ALA B 227 -39.008 74.861 23.822 1.00 38.6 ATOM 137 CB ALA B 227 -39.008 74.861 23.822 1.00 38.6 ATOM 138 C ALA B 227 -39.008 74.861 23.822 1.00 38.6 ATOM 140 N ALA B 227 -39.914 75.631 24.785 1.00 38.6 ATOM 140 N ALA B 228 -37.677 76.572 22.785 1.00 32.6 ATOM 140 N ALA B 228 -37.216 77.483 21.753 1.00 32.6 ATOM 140 CA ALA B 228 -37.216 77.483 21.753 1.00 32.6 ATOM 140 CA ALA B 228 -37.216 77.483 21.753 1.00 32.6 ATOM 140 CA ALA B 228 -37.216 77.483 21.753 1.00 32.6 ATOM 140 CA ALA B 228 -37.216 77.483 21.753 1.00 32.6 ATOM 140 CA ALA B 228 -37.216 77.483 21.753 1.00 32.6 ATOM 140 CA ALA B 228 -37.216 77.483 21.753 1.00 32.6 ATOM 140 CA ALA B 228 -37.216 77.483 21.753 1.00 32.6 ATOM 140 CA ALA B 228 -37.216 77.483 21.753 1.00 32.6 ATOM 140 CA ALA B 228 -37.216 77.483 21.753 1.00 32.6 ATOM 140 CA ALA B 228 -37.216 77.483 21.753 1.00 32.6 ATOM 140 CA ALA B 228 -37.216 77.483 21.753 1.00 32.6 ATOM 140 CA ALA B 228 -37.216 77.483 21.753 1.00 32.6 ATOM 140 CA ALA B 228 -37.216 77.483 21.753 1.00 32.6 ATOM 140 CA ALA B 228 -37.216 77.483 21.753 1.00 32.6 ATOM 140 CA ALA B 230 -36.545 77.483 1.9863 1.00 42.6 ATOM 140 CA ALA B 231 -39.353 72.30 72.30 1.00 44.6														
ATOM 126 C VAL B 225		5	ATOM	123	CB	VAL	В	225	-32.869	77.015	26.348	1.00	38.19	6
ATOM 126 C VAL B 225			ATOM	124	CG1	VAL	В	225	-31.863	76.983	25.226	1.00	36.77	6
ATOM 128 N THE B 226			ATOM	125	CG2	VAL	В	225	-32.483	78.050	27.353	1.00	41.76	6
ATOM 127			ATOM	126	С	VAL	В	225	-34.656	76.191	24.843	1.00	37.52	6
10						VAL	В	225	-34.621	76.364	23.638	1.00	36.77	8
ATOM 129 CA THR B 226		10							-35.005	75.046	25.410	1.00	34.02	7
ATOM 130 CB THR B 226									-35.423	73.887	24.638	1.00	34.67	6
ATOM 131 OG1 THR B 226									-35.677	72.707	25.574	1.00	30.56	6
ATOM 132 CG2 THR B 226										72.225	26.084	1.00	32.20	8
15 ATOM 134 C THR B 226												1.00	20.99	6
ATOM 134 O THR B 226		15										1.00	36.41	6
ATOM 135 N ALA B 227 -37.746 74.542 24.480 1.00 39.2 ATOM 136 CA ALA B 227 -39.008 74.861 23.822 1.00 36.5 ATOM 137 CB ALA B 227 -39.014 75.631 24.785 1.00 38.5 ATOM 139 O ALA B 227 -38.686 75.719 22.608 1.00 37.6 ATOM 139 O ALA B 227 -38.686 75.719 22.608 1.00 37.6 ATOM 140 N ALA B 228 -37.677 76.572 22.785 1.00 32.6 ATOM 141 CA ALA B 228 -37.216 77.483 21.753 1.00 32.6 ATOM 142 CB ALA B 228 -36.525 78.458 22.358 1.00 32.6 ATOM 143 C ALA B 228 -36.545 76.704 20.638 1.00 36.5 ATOM 144 O ALA B 228 -36.545 76.704 20.638 1.00 36.5 ATOM 145 N HIS B 229 -35.644 76.175 20.924 1.00 37.6 ATOM 145 N HIS B 229 -34.611 75.409 19.956 1.00 32.6 ATOM 147 CB HIS B 229 -33.418 74.721 20.597 1.00 32.6 ATOM 149 CD2 HIS B 229 -32.776 73.714 19.715 1.00 28.2 ATOM 149 CD2 HIS B 229 -32.535 72.384 19.863 1.00 28.2 ATOM 150 ND1 HIS B 229 -32.336 74.030 18.426 1.00 30.6 ATOM 150 ND1 HIS B 229 -32.535 72.384 19.863 1.00 28.2 ATOM 151 CE1 HIS B 229 -31.867 72.929 17.855 1.00 26.2 ATOM 153 C HIS B 229 -31.867 72.929 17.855 1.00 26.2 ATOM 155 N VAL B 230 -36.296 73.688 19.882 1.00 38.4 ATOM 156 CA VAL B 230 -36.296 73.688 19.882 1.00 38.4 ATOM 156 CA VAL B 230 -36.296 73.688 19.882 1.00 38.4 ATOM 157 CB VAL B 230 -36.296 73.688 19.882 1.00 38.4 ATOM 156 CA VAL B 230 -37.774 71.747 20.310 1.00 40.4 ATOM 157 CB VAL B 230 -38.374 71.311 18.045 1.00 41.5 ATOM 160 C VAL B 230 -38.375 72.505 17.248 1.00 40.4 ATOM 157 CB VAL B 230 -38.375 72.505 17.248 1.00 40.4 ATOM 161 O VAL B 230 -38.375 72.505 17.248 1.00 40.4 ATOM 166 C ALA B 231 -39.820 74.804 17.792 1.00 47.5 ATOM 166 CA ALA B 231 -39.820 74.804 17.792 1.00 47.5 ATOM 167 N THR B 232 -37.497 77.746 16.315 1.00 41.5 ATOM 167 N THR B 232 -37.914 75.773 16.669 1.00 47.5 ATOM 169 CB THR B 232 -37.914 75.773 16.669 1.00 47.5 ATOM 169 CB THR B 232 -37.924 75.774 16.6315 1.00 41.5 ATOM 169 CB THR B 232 -37.924 77.746 16.315 1.00 41.5 ATOM 170 OGI THR B 232 -37.924 75.779 14.914 1.00 43.5 ATOM 170 OGI THR B 232 -37.943 77.746 16.315 1.00 41.5 ATOM 172 C THR B 232 -37.943 77.746 16.315 1.00 41.5 AT		13												8
ATOM 136 CA ALA B 227 -39.008 74.861 23.822 1.00 36.5 ATOM 137 CB ALA B 227 -39.914 75.631 24.785 1.00 38.0 ATOM 138 C ALA B 227 -39.914 75.631 24.785 1.00 38.0 ATOM 138 C ALA B 227 -39.317 75.616 21.566 1.00 40.5 ATOM 140 N ALA B 228 -37.677 76.572 22.785 1.00 32.6 ATOM 141 CA ALA B 228 -37.216 77.483 21.753 1.00 32.6 ATOM 142 CB ALA B 228 -36.252 78.458 22.358 1.00 28.2 ATOM 144 C ALA B 228 -36.545 76.704 20.638 1.00 36.1 ATOM 145 N HIS B 228 -36.545 76.704 20.638 1.00 36.1 ATOM 145 N HIS B 229 -35.364 76.175 20.924 1.00 37.3 ATOM 146 CA HIS B 229 -35.364 76.175 20.924 1.00 37.3 ATOM 147 CB HIS B 229 -33.418 74.721 20.597 1.00 33.4 ATOM 149 CD2 HIS B 229 -32.776 73.714 19.715 1.00 28.3 ATOM 149 CD2 HIS B 229 -32.336 74.030 18.426 1.00 28.3 ATOM 150 ND1 HIS B 229 -32.336 74.030 18.426 1.00 28.3 ATOM 151 CE1 HIS B 229 -32.336 74.030 18.426 1.00 30.4 ATOM 151 CE1 HIS B 229 -31.867 72.929 17.855 1.00 26.5 ATOM 155 N VAL B 230 -35.362 74.352 19.202 1.00 38.4 ATOM 156 CA VAL B 230 -35.62 74.351 18.045 1.00 41.4 ATOM 156 CA VAL B 230 -36.296 73.688 19.882 1.00 38.4 ATOM 156 CA VAL B 230 -37.774 71.747 20.310 1.00 41.4 ATOM 159 CC2 VAL B 230 -38.381 70.537 19.637 1.00 40.4 ATOM 159 CC2 VAL B 230 -37.774 71.747 20.310 1.00 44.4 ATOM 160 C VAL B 230 -38.381 70.537 19.637 1.00 40.4 ATOM 161 O VAL B 230 -38.381 70.537 19.637 1.00 40.4 ATOM 162 N ALA B 231 -39.827 74.351 18.645 1.00 45.5 ATOM 166 C ALA B 231 -39.827 74.351 18.645 1.00 40.4 ATOM 167 N THR B 232 -37.744 71.747 20.310 1.00 44.4 ATOM 168 CA THR B 231 -39.827 77.746 16.315 1.00 41.5 ATOM 169 CB THR B 232 -37.744 77.746 16.315 1.00 41.5 ATOM 169 CB THR B 232 -37.744 77.746 16.315 1.00 41.5 ATOM 169 CB THR B 232 -37.914 75.773 16.669 1.00 47.5 ATOM 169 CB THR B 232 -36.402 77.746 16.315 1.00 41.5 ATOM 169 CB THR B 232 -36.402 77.746 16.315 1.00 41.5 ATOM 170 OGI THR B 232 -36.402 77.746 16.315 1.00 41.5 ATOM 171 CG2 THR B 232 -36.401 76.252 14.155 1.00 40.5 ATOM 173 O THR B 232 -36.401 76.252 14.155 1.00 40.5 ATOM 175 CA ASN B 233 -36.5195 74.407 15.1575 1.00 40														7
ATOM 137 CB ALA B 227 -39.914 75.631 24.785 1.00 38.0 ATOM 138 C ALA B 227 -38.686 75.719 22.608 1.00 37.6 ATOM 140 N ALA B 227 -38.317 75.616 21.566 1.00 40.5 ATOM 141 CA ALA B 228 -37.216 77.483 21.753 1.00 32.6 ATOM 141 CA ALA B 228 -37.216 77.483 21.753 1.00 32.6 ATOM 142 CB ALA B 228 -37.216 77.483 21.753 1.00 32.6 ATOM 144 C ALA B 228 -36.545 76.704 20.638 1.00 28.6 ATOM 145 N HIS B 229 -35.364 76.175 20.924 1.00 37.6 ATOM 146 CA HIS B 229 -33.364 76.175 20.924 1.00 37.6 ATOM 147 CB HIS B 229 -33.418 74.721 20.597 1.00 33.6 ATOM 149 CD2 HIS B 229 -32.776 73.714 19.715 1.00 28.6 ATOM 150 ND1 HIS B 229 -32.535 72.384 19.863 1.00 28.6 ATOM 150 ND1 HIS B 229 -31.867 72.929 17.855 1.00 28.6 ATOM 150 ND1 HIS B 229 -31.867 72.929 17.855 1.00 28.6 ATOM 150 ND1 HIS B 229 -35.069 74.131 18.045 1.00 31.6 ATOM 150 ND1 B 230 -37.744 71.747 20.310 1.00 31.6 ATOM 150 NA B 230 -37.744 71.747 20.310 1.00 38.4 ATOM 150 NA B 230 -37.744 71.747 20.310 1.00 40.6 ATOM 150 CA VAL B 230 -37.744 71.747 20.310 1.00 40.6 ATOM 150 CA VAL B 230 -37.744 71.747 20.310 1.00 44.6 ATOM 150 CA VAL B 230 -38.313 70.537 19.637 1.00 40.6 ATOM 150 CA VAL B 230 -38.313 70.537 19.637 1.00 40.6 ATOM 160 C VAL B 230 -38.313 70.537 19.637 1.00 44.6 ATOM 161 CO VAL B 230 -38.744 71.747 20.310 1.00 44.6 ATOM 166 CA ALA B 231 -39.825 75.636 16.63 1.00 40.6 ATOM 166 CA ALA B 231 -39.825 75.636 16.63 1.00 40.6 ATOM 167 N THR B 232 -37.744 71.747 20.310 1.00 44.6 ATOM 168 CA BLA B 231 -39.825 75.636 16.63 1.00 40.6 ATOM 167 N THR B 232 -37.744 77.746 16.315 1.00 47.6 ATOM 168 CA THR B 232 -37.914 75.773 16.669 1.00 47.6 ATOM 167 N THR B 232 -37.914 75.773 16.669 1.00 49.6 ATOM 167 N THR B 232 -37.914 75.773 16.669 1.00 49.6 ATOM 167 N THR B 232 -37.914 75.773 16.669 1.00 49.6 ATOM 167 N THR B 232 -37.914 75.773 16.669 1.00 49.6 ATOM 167 N THR B 232 -37.914 75.773 16.669 1.00 49.6 ATOM 167 N THR B 232 -37.914 75.773 16.669 1.00 49.6 ATOM 167 N THR B 232 -37.914 75.773 16.669 1.00 49.6 ATOM 170 CGI THR B 232 -37.914 75.														6
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ATOM 155 N VAL B 230 -36.296 73.688 19.882 1.00 38.2 ATOM 155 N VAL B 230 -37.077 72.634 19.263 1.00 38.2 ATOM 157 CB VAL B 230 -37.744 71.747 20.310 1.00 40.4 ATOM 158 CG1 VAL B 230 -38.381 70.537 19.637 1.00 39.3 ATOM 159 CG2 VAL B 230 -38.381 70.537 19.637 1.00 39.3 ATOM 160 C VAL B 230 -38.381 70.537 19.637 1.00 42.3 ATOM 161 O VAL B 230 -38.375 72.505 17.248 1.00 45.5 ATOM 162 N ALA B 231 -38.774 74.240 18.623 1.00 45.5 ATOM 163 CA ALA B 231 -38.774 74.240 18.623 1.00 45.5 ATOM 164 CB ALA B 231 -38.277 48.04 17.792 1.00 47.3 ATOM 165 C ALA B 231 -39.20 74.804 17.792 1.00 47.3 ATOM 166 O ALA B 231 -39.25 75.636 16.673 1.00 45.5 ATOM 166 O ALA B 231 -39.25 75.636 16.673 1.00 45.5 ATOM 167 N THR B 232 -37.240 76.563 15.654 1.00 49.5 ATOM 168 CA THR B 232 -37.914 75.773 16.669 1.00 47.3 ATOM 169 CB THR B 232 -37.240 76.563 15.654 1.00 49.3 ATOM 169 CB THR B 232 -37.240 76.563 15.654 1.00 49.3 ATOM 170 OG1 THR B 232 -36.482 77.746 16.315 1.00 41.5 ATOM 170 CG1 THR B 232 -36.482 77.746 16.315 1.00 41.5 ATOM 171 CG2 THR B 232 -36.482 77.746 16.315 1.00 41.5 ATOM 172 C THR B 232 -36.194 75.779 17.998 1.00 39.3 ATOM 172 C THR B 232 -36.194 75.779 17.998 1.00 39.3 ATOM 173 O THR B 232 -36.194 75.779 17.998 1.00 39.3 ATOM 173 O THR B 232 -36.194 75.779 17.998 1.00 39.3 ATOM 173 O THR B 232 -36.194 75.779 17.998 1.00 49.4 ATOM 175 CA ASN B 233 -36.195 74.407 15.155 1.00 40.5 ATOM 175 CA ASN B 233 -36.195 74.407 15.155 1.00 40.5 ATOM 175 CA ASN B 233 -35.247 73.511 14.483 1.00 58.4	1.1				NE2									7
ATOM 155 N VAL B 230 -36.296 73.688 19.882 1.00 38.2 ATOM 155 N VAL B 230 -37.077 72.634 19.263 1.00 38.2 ATOM 157 CB VAL B 230 -37.744 71.747 20.310 1.00 40.4 ATOM 158 CG1 VAL B 230 -38.381 70.537 19.637 1.00 39.3 ATOM 159 CG2 VAL B 230 -38.381 70.537 19.637 1.00 39.3 ATOM 160 C VAL B 230 -38.381 70.537 19.637 1.00 42.3 ATOM 161 O VAL B 230 -38.375 72.505 17.248 1.00 45.5 ATOM 162 N ALA B 231 -38.774 74.240 18.623 1.00 45.5 ATOM 163 CA ALA B 231 -38.774 74.240 18.623 1.00 45.5 ATOM 164 CB ALA B 231 -38.277 48.04 17.792 1.00 47.3 ATOM 165 C ALA B 231 -39.20 74.804 17.792 1.00 47.3 ATOM 166 O ALA B 231 -39.25 75.636 16.673 1.00 45.5 ATOM 166 O ALA B 231 -39.25 75.636 16.673 1.00 45.5 ATOM 167 N THR B 232 -37.240 76.563 15.654 1.00 49.5 ATOM 168 CA THR B 232 -37.914 75.773 16.669 1.00 47.3 ATOM 169 CB THR B 232 -37.240 76.563 15.654 1.00 49.3 ATOM 169 CB THR B 232 -37.240 76.563 15.654 1.00 49.3 ATOM 170 OG1 THR B 232 -36.482 77.746 16.315 1.00 41.5 ATOM 170 CG1 THR B 232 -36.482 77.746 16.315 1.00 41.5 ATOM 171 CG2 THR B 232 -36.482 77.746 16.315 1.00 41.5 ATOM 172 C THR B 232 -36.194 75.779 17.998 1.00 39.3 ATOM 172 C THR B 232 -36.194 75.779 17.998 1.00 39.3 ATOM 173 O THR B 232 -36.194 75.779 17.998 1.00 39.3 ATOM 173 O THR B 232 -36.194 75.779 17.998 1.00 39.3 ATOM 173 O THR B 232 -36.194 75.779 17.998 1.00 49.4 ATOM 175 CA ASN B 233 -36.195 74.407 15.155 1.00 40.5 ATOM 175 CA ASN B 233 -36.195 74.407 15.155 1.00 40.5 ATOM 175 CA ASN B 233 -35.247 73.511 14.483 1.00 58.4	518.5	35	MOTA											6
ATOM 156 CA VAL B 230 -37.77 72.634 19.263 1.00 40.4 4.6 ATOM 157 CB VAL B 230 -37.744 71.747 20.310 1.00 44.6 ATOM 158 CG1 VAL B 230 -38.381 70.537 19.637 1.00 39.5 ATOM 159 CG2 VAL B 230 -36.742 71.311 21.356 1.00 40.4 ATOM 159 CG2 VAL B 230 -36.742 71.311 21.356 1.00 42.5 ATOM 160 C VAL B 230 -38.133 73.130 18.284 1.00 44.5 ATOM 161 O VAL B 230 -38.375 72.505 17.248 1.00 45.5 ATOM 162 N ALA B 231 -38.774 74.240 18.623 1.00 45.5 ATOM 164 CB ALA B 231 -39.820 74.804 17.792 1.00 47.6 ATOM 165 C ALA B 231 -39.820 74.804 17.792 1.00 47.6 ATOM 166 O ALA B 231 -39.235 75.636 16.673 1.00 45.6 ATOM 167 N THR B 232 -37.914 75.763 15.666 10.00 49.5 ATOM 168 CA THR B 232 -37.914 75.774 16.669 1.00 47.6 ATOM 168 CA THR B 232 -37.914 75.774 16.669 1.00 47.6 ATOM 169 CB THR B 232 -37.914 75.774 16.659 1.00 47.6 ATOM 170 OG1 THR B 232 -35.385 77.270 17.098 1.00 39.6 ATOM 171 CG2 THR B 232 -35.385 77.270 17.098 1.00 39.6 ATOM 172 C THR B 232 -36.482 77.746 16.315 1.00 41.5 ATOM 172 C THR B 232 -36.492 77.746 16.315 1.00 41.5 ATOM 173 O THR B 232 -35.401 76.252 14.155 1.00 40.5 ATOM 174 N ASN B 233 -36.194 75.779 14.914 1.00 43.5 ATOM 174 N ASN B 233 -36.195 74.407 15.515 1.00 40.5 ATOM 175 CA ASN B 233 -35.247 73.511 14.483 1.00 58.4	177		ATOM	154	0									8
ATOM 156 CA VAL B 230 -37.744 71.747 20.310 1.00 44.54 40 ATOM 157 CB VAL B 230 -38.381 70.537 19.637 1.00 43.54 ATOM 159 CG2 VAL B 230 -38.381 70.537 19.637 1.00 42.54 ATOM 160 C VAL B 230 -38.133 73.130 18.284 1.00 42.54 ATOM 161 O VAL B 230 -38.133 73.130 18.284 1.00 44.54 ATOM 162 N ALAB 231 -38.375 72.505 17.248 1.00 45.54 ATOM 163 CA ALAB 231 -39.820 74.804 17.792 1.00 47.54 ATOM 164 CB ALAB 231 -39.820 74.804 17.792 1.00 47.54 ATOM 165 C ALAB 231 -39.820 74.804 17.792 1.00 47.54 ATOM 166 O ALAB 231 -39.959 75.636 16.673 1.00 45.54 ATOM 167 N THR B 232 -37.914 75.773 16.669 1.00 49.54 ATOM 168 CA THR B 232 -37.914 75.773 16.669 1.00 47.55 ATOM 169 CB THR B 232 -36.482 77.746 16.315 1.00 41.54 ATOM 170 OG1 THR B 232 -36.482 77.746 16.315 1.00 41.54 ATOM 171 CG2 THR B 232 -36.482 77.745 16.315 1.00 41.55 ATOM 172 C THR B 232 -36.194 75.779 14.914 1.00 43.55 ATOM 173 O THR B 232 -36.194 75.779 14.914 1.00 43.55 ATOM 174 N ASN B 233 -36.195 74.407 15.157 1.00 40.55 ATOM 175 CA ASN B 233 -35.247 73.511 14.483 1.00 58.45			ATOM	155	N									7
40 ATOM 158 CG1 VAL B 230 -38.381 70.537 19.637 1.00 39.1 ATOM 159 CG2 VAL B 230 -36.742 71.311 21.356 1.00 42.1 ATOM 160 C VAL B 230 -38.133 73.130 18.284 1.00 42.1 ATOM 161 O VAL B 230 -38.375 72.505 17.248 1.00 45.5 ATOM 162 N ALA B 231 -38.774 74.240 18.623 1.00 45.5 ATOM 163 CA ALA B 231 -39.820 74.804 17.792 1.00 47.3 ATOM 164 CB ALA B 231 -40.736 75.661 18.647 1.00 45.0 ATOM 165 C ALA B 231 -39.820 74.804 17.792 1.00 47.3 ATOM 166 O ALA B 231 -39.959 76.128 15.816 1.00 49.0 ATOM 167 N THR B 232 -37.914 75.773 16.669 1.00 47.3 ATOM 168 CA THR B 232 -37.914 75.773 16.669 1.00 47.3 ATOM 169 CB THR B 232 -37.220 76.563 15.654 1.00 49.0 ATOM 170 OG1 THR B 232 -36.482 77.746 16.315 1.00 41.3 ATOM 171 CG2 THR B 232 -37.423 78.523 17.221 1.00 29.8 ATOM 172 C THR B 232 -36.194 75.779 14.914 1.00 43.3 ATOM 173 O THR B 232 -36.194 75.779 14.914 1.00 43.3 ATOM 174 N ASN B 233 -36.195 74.407 15.157 1.00 40.3 ATOM 175 CA ASN B 233 -36.195 74.407 15.157 1.00 40.3 ATOM 174 N ASN B 233 -36.195 74.407 15.157 1.00 40.5 ATOM 175 CA ASN B 233 -35.247 73.511 14.483 1.00 58.4	122		ATOM	156	CA	VAL	В	230						6
ATOM 159 CG2 VAL B 230 -36.742 71.311 21.356 1.00 42.1 ATOM 160 C VAL B 230 -38.133 73.130 18.284 1.00 44.2 ATOM 161 O VAL B 230 -38.375 72.505 17.248 1.00 45.4 ATOM 162 N ALA B 231 -38.774 74.240 18.623 1.00 45.4 ATOM 163 CA ALA B 231 -39.820 74.804 17.792 1.00 45.4 ATOM 165 C ALA B 231 -39.820 74.804 17.792 1.00 45.4 ATOM 165 C ALA B 231 -39.235 75.636 16.673 1.00 48.6 ATOM 166 O ALA B 231 -39.235 75.636 15.673 1.00 48.6 ATOM 167 N THR B 232 -37.220 76.563 15.654 1.00 49.5 ATOM 168 CA THR B 232 -37.220 76.563 15.654 1.00 49.5 ATOM 169 CB THR B 232 -37.220 76.563 15.654 1.00 43.4 ATOM 170 OG1 THR B 232 -37.423 78.523 17.232 1.00 29.6 ATOM 171 CG2 THR B 232 -37.423 78.523 17.232 1.00 29.6 ATOM 172 C THR B 232 -36.482 77.746 16.315 1.00 41.5 ATOM 173 O THR B 232 -37.423 78.523 17.232 1.00 29.6 ATOM 174 N ASN B 233 -36.194 75.719 14.914 1.00 43.4 ATOM 175 CA ASN B 233 -35.247 73.511 14.483 1.00 58.4			ATOM	157	CB	VAL	В	230	-37.744	71.747				6
ATOM 160 C VAL B 230 -38.133 73.130 18.284 1.00 44.2 ATOM 161 O VAL B 230 -38.375 72.505 17.248 1.00 45.9 ATOM 162 N ALA B 231 -38.774 74.240 18.623 1.00 45.9 45 ATOM 163 CA ALA B 231 -39.820 74.804 17.792 1.00 47.8 ATOM 164 CB ALA B 231 -40.736 75.661 18.647 1.00 45.0 ATOM 165 C ALA B 231 -39.235 75.636 16.673 1.00 45.0 ATOM 166 O ALA B 231 -39.959 76.128 15.816 1.00 49.9 ATOM 167 N THR B 232 -37.914 75.773 16.669 1.00 47.8 ATOM 168 CA THR B 232 -37.914 75.773 16.669 1.00 47.8 ATOM 169 CB THR B 232 -37.20 76.563 15.641 1.00 47.8 ATOM 170 OGI THR B 232 -35.365 77.270 17.098 1.00 39.3 ATOM 171 CG2 THR B 232 -36.482 77.746 16.315 1.00 41.9 ATOM 172 C THR B 232 -36.194 75.779 14.914 1.00 43.9 ATOM 173 O THR B 232 -36.194 75.719 14.914 1.00 43.9 ATOM 174 N ASN B 233 -36.195 74.407 15.155 1.00 40.3 ATOM 175 CA ASN B 233 -35.247 73.511 14.483 1.00 58.4		40	ATOM	158	CG1	VAL	В	230						6
ATOM 161 O VAL B 230 -38.375 72.505 17.248 1.00 45.5 ATOM 162 N ALA B 231 -38.774 74.240 18.623 1.00 45.5 45 ATOM 163 CA ALA B 231 -38.20 74.804 17.792 1.00 47.5 ATOM 164 CB ALA B 231 -40.736 75.661 18.647 1.00 45.5 ATOM 165 C ALA B 231 -39.235 75.636 16.673 1.00 48.6 ATOM 166 O ALA B 231 -39.959 76.128 15.816 1.00 49.5 ATOM 167 N THR B 232 -37.914 75.773 16.669 1.00 47.5 50 ATOM 168 CA THR B 232 -37.220 76.563 15.654 1.00 41.0 ATOM 169 CB THR B 232 -36.482 77.746 16.315 1.00 41.5 ATOM 170 OGI THR B 232 -36.482 77.746 16.315 1.00 41.5 ATOM 171 CG2 THR B 232 -37.423 78.523 17.232 1.00 29.5 ATOM 172 C THR B 232 -36.194 75.779 14.914 1.00 43.5 ATOM 173 O THR B 232 -36.194 75.779 14.914 1.00 43.5 55 ATOM 173 O THR B 232 -36.194 75.719 14.914 1.00 43.5 ATOM 174 N ASN B 233 -36.195 74.407 15.155 1.00 40.5 ATOM 175 CA ASN B 233 -35.247 73.511 14.483 1.00 58.4			ATOM	159	CG2	VAL	В	230	-36.742	71.311				6
ATOM 162 N ALA B 231 -38.774 74.240 18.623 1.00 45.1 45 ATOM 163 CA ALA B 231 -39.820 74.804 17.792 1.00 47.8 ATOM 164 CB ALA B 231 -39.820 74.804 17.792 1.00 47.8 ATOM 165 C ALA B 231 -39.235 75.636 16.673 1.00 48.0 ATOM 166 O ALA B 231 -39.959 76.128 15.816 1.00 49.9 ATOM 167 N THR B 232 -37.914 75.773 16.669 1.00 47.2 50 ATOM 168 CA THR B 232 -37.220 76.563 15.654 1.00 43.9 ATOM 169 CB THR B 232 -37.220 76.563 15.654 1.00 43.9 ATOM 170 OGI THR B 232 -35.855 77.270 17.098 1.00 39.2 ATOM 171 CG2 THR B 232 -37.423 78.523 17.232 1.00 29.8 ATOM 172 C THR B 232 -36.194 75.719 14.914 1.00 43.9 ATOM 173 O THR B 232 -36.194 75.719 14.914 1.00 43.9 ATOM 174 N ASN B 233 -36.195 74.407 15.157 1.00 48.4 ATOM 175 CA ASN B 233 -35.247 73.511 14.483 1.00 58.4			ATOM	160	C	VAL	В	230	-38.133					6
45 ATOM 163 CA ALA B 231 -39.820 74.804 17.792 1.00 47.4 ATOM 164 CB ALA B 231 -40.736 75.661 18.647 1.00 45.4 ATOM 165 C ALA B 231 -39.235 75.661 18.647 1.00 45.4 ATOM 166 O ALA B 231 -39.959 76.128 15.816 1.00 49.5 ATOM 167 N THR B 232 -37.914 75.773 16.669 1.00 47.5 50 ATOM 168 CA THR B 232 -37.914 75.773 16.669 1.00 47.5 ATOM 169 CB THR B 232 -36.482 77.746 16.315 1.00 41.5 ATOM 170 OGI THR B 232 -35.385 77.270 17.098 1.00 41.5 ATOM 171 CG2 THR B 232 -36.482 77.746 16.315 1.00 41.5 ATOM 172 C THR B 232 -36.194 75.779 14.914 1.00 43.5 55 ATOM 173 O THR B 232 -35.401 76.252 14.155 1.00 40.5 ATOM 174 N ASN B 233 -36.195 74.407 15.157 1.00 40.5 ATOM 175 CA ASN B 233 -35.247 73.511 14.483 1.00 58.4			ATOM	161	0	VAL	В	230	-38.375	72.505	17.248	1.00	45.94	8
ATOM 164 CB ALA B 231 -40.736 75.661 18.647 1.00 45.0 ATOM 165 C ALA B 231 -39.235 75.636 16.673 1.00 45.0 ATOM 166 O ALA B 231 -39.959 76.128 15.816 1.00 49.0 ATOM 167 N THR B 232 -37.914 75.773 16.669 1.00 47.3 50 ATOM 168 CA THR B 232 -37.220 76.563 15.654 1.00 43.0 ATOM 169 CB THR B 232 -36.482 77.746 16.315 1.00 41.3 ATOM 170 OGI THR B 232 -36.482 77.746 16.315 1.00 41.3 ATOM 171 CG2 THR B 232 -35.385 77.270 17.098 1.00 39.3 ATOM 171 CG2 THR B 232 -36.194 75.719 14.914 1.00 43.3 ATOM 172 C THR B 232 -36.194 75.719 14.914 1.00 43.3 55 ATOM 173 O THR B 232 -36.194 75.719 14.914 1.00 43.3 ATOM 175 CA ASN B 233 -36.195 74.407 15.157 1.00 40.3 ATOM 175 CA ASN B 233 -35.247 73.511 14.483 1.00 58.4			ATOM	162	N	ALA	В	231	-38.774	74.240	18.623	1.00	45.59	7
ATOM 165 C ALA B 231 -39.235 75.636 16.673 1.00 48.0 ATOM 166 O ALA B 231 -39.959 76.128 15.816 1.00 49.9 ATOM 167 N THR B 232 -37.914 75.773 16.669 1.00 49.9 STOR ATOM 168 CA THR B 232 -37.220 76.563 15.654 1.00 43.0 ATOM 169 CB THR B 232 -36.482 77.746 16.315 1.00 41.9 ATOM 170 OGI THR B 232 -35.385 77.270 17.098 1.00 39.0 ATOM 171 CG2 THR B 232 -37.423 78.523 17.232 1.00 29.0 ATOM 172 C THR B 232 -37.423 78.523 17.232 1.00 29.0 ATOM 173 O THR B 232 -36.194 75.719 14.914 1.00 43.0 ATOM 174 N ASN B 233 -36.195 74.407 15.157 1.00 48.0 ATOM 175 CA ASN B 233 -35.247 73.511 14.483 1.00 58.0		45	ATOM	163	CA	ALA	В	231	-39.820	74.804	17.792	1.00	47.84	6
ATOM 166 C ALA B 231 -39.235 75.636 16.673 1.00 48.0 ATOM 166 O ALA B 231 -39.959 76.128 15.816 1.00 49.0 ATOM 167 N THR B 232 -37.914 75.773 16.669 1.00 47.0 50 ATOM 168 CA THR B 232 -37.220 76.563 15.654 1.00 43.0 ATOM 169 CB THR B 232 -36.482 77.746 16.315 1.00 41.0 ATOM 170 OG1 THR B 232 -35.385 77.270 17.098 1.00 39.0 ATOM 171 CG2 THR B 232 -37.423 78.523 17.232 1.00 29.0 ATOM 172 C THR B 232 -37.423 78.523 17.232 1.00 29.0 ATOM 173 O THR B 232 -36.194 75.719 14.914 1.00 43.0 ATOM 174 N ASN B 233 -36.195 74.407 15.157 1.00 48.0 ATOM 175 CA ASN B 233 -35.247 73.511 14.483 1.00 58.0			ATOM	164	CB	ALA	В	231	-40.736	75.661	18.647	1.00	45.08	6
ATOM 166 O ALA B 231 -39,959 76.128 15.816 1.00 49.5 50 ATOM 168 CA THR B 232 -37.220 76.563 15.654 1.00 47.2 ATOM 168 CA THR B 232 -37.220 76.563 15.654 1.00 47.2 ATOM 170 OGI THR B 232 -36.482 77.746 16.315 1.00 41.5 ATOM 171 CG2 THR B 232 -35.385 77.270 17.098 1.00 39.3 ATOM 172 C THR B 232 -37.423 78.523 17.232 1.00 29.5 ATOM 173 O THR B 232 -36.194 75.719 14.914 1.00 43.5 55 ATOM 173 O THR B 232 -35.401 76.252 14.155 1.00 40.3 ATOM 174 N ASN B 233 -36.195 74.407 15.157 1.00 48.3 ATOM 175 CA ASN B 233 -35.247 73.511 14.483 1.00 58.4					С	ALA	В	231	-39.235	75.636	16.673	1.00	48.04	6
ATOM 167 N THR B 232 -37.914 75.773 16.669 1.00 47.5 ATOM 168 CA THR B 232 -37.220 76.563 15.654 1.00 43.4 ATOM 169 CB THR B 232 -36.482 77.746 16.315 1.00 41.5 ATOM 170 OGI THR B 232 -36.482 77.746 16.315 1.00 41.5 ATOM 171 CG2 THR B 232 -35.385 77.270 17.098 1.00 39.3 ATOM 172 C THR B 232 -37.423 78.523 17.232 1.00 29.8 ATOM 173 O THR B 232 -36.194 75.719 14.914 1.00 43.3 55 ATOM 173 O THR B 232 -35.401 76.252 14.155 1.00 40.3 ATOM 175 CA ASN B 233 -36.195 74.407 15.157 1.00 48.3 ATOM 175 CA ASN B 233 -35.247 73.511 14.483 1.00 58.4					0	ALA	В	231	-39.959	76.128	15.816	1.00	49.95	8
50 ATOM 168 CA THR B 232 -37.220 76.563 15.664 1.00 43.4 ATOM 169 CB THR B 232 -36.482 77.746 16.315 1.00 41.5 ATOM 170 OG1 THR B 232 -35.385 77.270 17.098 1.00 39.5 ATOM 171 CG2 THR B 232 -37.423 78.523 17.232 1.00 29.6 ATOM 172 C THR B 232 -36.194 75.719 14.914 1.00 43.5 ATOM 173 O THR B 232 -36.194 75.719 14.914 1.00 43.5 ATOM 174 N ASN B 233 -36.195 74.407 15.157 1.00 48.5 ATOM 175 CA ASN B 233 -35.247 73.511 14.483 1.00 58.7				167	N	THR	В	232	-37.914	75.773	16.669	1.00	47.26	7
ATOM 169 CB THR B 232 -36.482 77.746 16.315 1.00 41.5 ATOM 170 OG1 THR B 232 -35.385 77.270 17.098 1.00 39.1 ATOM 171 CG2 THR B 232 -37.423 78.523 17.232 1.00 29.5 ATOM 172 C THR B 232 -36.194 75.719 14.914 1.00 43.5 ATOM 173 O THR B 232 -35.401 76.252 14.155 1.00 40.5 ATOM 174 N ASN B 233 -36.195 74.407 15.157 1.00 48.5 ATOM 175 CA ASN B 233 -35.247 73.511 14.483 1.00 58.1		50		168	CA	THR	В	232	-37.220	76.563	15.654	1.00	43.64	6
ATOM 170 OG1 THR B 232 -35.385 77.270 17.098 1.00 39.1 ATOM 171 CG2 THR B 232 -37.423 78.523 17.232 1.00 29.8 ATOM 172 C THR B 232 -36.194 75.719 14.914 1.00 43.1 55 ATOM 173 O THR B 232 -35.401 76.252 14.155 1.00 40.1 ATOM 174 N ASN B 233 -36.195 74.407 15.157 1.00 48.1 ATOM 175 CA ASN B 233 -35.247 73.511 14.483 1.00 58.1						THR	В	232	-36.482	77.746	16.315	1.00	41.93	6
ATOM 171 CG2 THR B 232 -37.423 78.523 17.232 1.00 29.6 ATOM 172 C THR B 232 -36.194 75.719 14.914 1.00 43.5 55 ATOM 173 O THR B 232 -35.401 76.252 14.155 1.00 40.5 ATOM 174 N ASN B 233 -36.195 74.407 15.157 1.00 48.5 ATOM 175 CA ASN B 233 -35.247 73.511 14.483 1.00 58.6									-35.385	77.270	17.098	1.00	39.10	8
ATOM 172 C THR B 232 -36.194 75.719 14.914 1.00 43.1 55 ATOM 173 O THR B 232 -35.401 76.252 14.155 1.00 40.1 ATOM 174 N ASN B 233 -36.195 74.407 15.157 1.00 48.1 ATOM 175 CA ASN B 233 -35.247 73.511 14.483 1.00 58.1										78.523	17.232	1.00	29.80	6
55 ATOM 173 O THR B 232 -35.401 76.252 14.155 1.00 40.1 ATOM 174 N ASN B 233 -36.195 74.407 15.157 1.00 48.1 ATOM 175 CA ASN B 233 -35.247 73.511 14.483 1.00 58.1										75.719	14.914	1.00	43.97	6
ATOM 174 N ASN B 233 -36.195 74.407 15.157 1.00 48.0 ATOM 175 CA ASN B 233 -35.247 73.511 14.483 1.00 58.0		55												8
ATOM 175 CA ASN B 233 -35.247 73.511 14.483 1.00 58.		55												7
11011 170 011 11011 2 000														6
111011 170 00 1101 2 -01														6
			21 011	1,0	CD	11014	_	200	0					

	ATOM	177	CG	ASN	D	222	-33.407	71.812	14.946	1.00 68.3	5 6
							-32.569	72.427	14.256	1.00 65.5	
	ATOM	178		ASN				70.529	15.265	1.00 74.2	
	ATOM	179		ASN		233	-33.288			1.00 /4.2	-
	MOTA	180	С	ASN		233	-36.033	72.755	13.437		
	ATOM	181	0	ASN			-36.950	72.005	13.754	1.00 69.4	
10) ATOM	182	N	ALA		234	-35.674	72.986	12.182	1.00 68.8	
	ATOM	183	CA	ALA	В	234	-36.352	72.376	11.036	1.00 70.9	
	ATOM	184	CB	ALA	В	234	-35.585	72.701	9.769	1.00 71.4	
	ATOM	185	С	ALA	В	234	-36.556	70.880	11.111	1.00 73.8	
	ATOM	186	0	ALA	В	234	-35.677	70.142	11.501	1.00 74.3	3 8
1:	5 ATOM	187	N	GLN	В	235	-37.754	70.479	10.717	1.00 75.0	7 7
	ATOM	188	CA	GLN	В	235	-38.149	69.095	10.690	1.00 76.3	2 6
	ATOM	189	СВ	GLN	В	235	-37.468	68.365	9.533	1.00 76.9	8 6
	ATOM	190	CG	GLN		235	-38.120	68.540	8.170	1.00 77.0	7 6
	ATOM	191	CD	GLN		235	-38.572	69.940	7.909	1.00 80.8	5 6
20		192	OE1	GLN		235	-39.575	70.401	8.491	1.00 82.0	1 8
21	ATOM	193	NE2	GLN			-37.862	70.620	7.040	1.00 78.8	
	ATOM	194	C	GLN			-37.904	68.331	11.953	1.00 77.1	
		194	0	GLN		235	-38.087	67.137	11.947	1.00 76.0	
(200)	ATOM			GLY			-37.511	68.985	13.039	1.00 77.4	
© 2	ATOM	196	N	GLY			-37.304	68.263	14.288	1.00 78.3	
10 2:		197	CA				-36.717	66.882	14.217	1.00 70.4	
10	ATOM	198	С	GLY		236		66.650	13.542	1.00 79.4	
hala hala	ATOM	199	0	GLY		236	-35.717 -37.420	66.007	14.943	1.00 77.9	
See See	ATOM	200	N	SER		237				1.00 77.3	
4 4	MOTA	201	CA	SER			-37.117	64.600	15.092	1.00 76.4	
3		202	CB	SER			-38.118	63.953	16.066		
6)	ATOM	203	С	SER			-37.181	63.895	13.737	1.00 75.3	
	ATOM	204	0	SER		237	-36.493	62.911	13.524	1.00 75.4	
	ATOM	205	N	HIS			-38.004	64.443	12.845	1.00 75.5	
a 3	ATOM	206	CA	HIS			-38.293	63.926	11.519	1.00 75.4	
1AJ 3		207	CB	HIS		238	-39.663	64.397	11.096	1.00 75.8	
123	MOTA	208	С	HIS			-37.369	64.216	10.380	1.00 74.1	
ō	ATOM	209	0			238	-37.747	64.135	9.222	1.00 75.3	
-	MOTA	210	N			239	-36.127	64.427	10.651	1.00 73.3	
	ATOM	211	CA			239	-35.345	64.786	9.519	1.00 74.0	
4	MOTA 0	212	CB			239	-34.121	65.542	9.934	1.00 81.7	
	ATOM	213	CG			239	-33.085	64.786	10.737	1.00 89.6	
	ATOM	214	CD2				-31.727	64.530	10.302	1.00 93.1	
	MOTA	215	CE2	TRP	В	239	-31.069	63.848	11.393	1.00 95.4	
	MOTA	216	CE3	TRP	В	239	-30.949	64.941	9.196	1.00 95.3	
4	5 ATOM	217	CD1	TRP	В	239	-33.237	64.180	11.926	1.00 94.1	
	ATOM	218	NE1	TRP	В	239	-32.022	63.631	12.347	1.00 97.4	
	ATOM	219	CZ2	TRP	В	239	-29.706	63.475	11.348	1.00 96.2	
	ATOM	220	CZ3	TRP	В	239	-29.613	64.533	9.128	1.00 96.7	
	ATOM	221	CH2	TRP	В	239	-28.978	63.870	10.215	1.00 97.3	32 6
5	MOTA 0	222	С	TRP	В	239	-34.994	63.722	8.539	1.00 70.	17 6
_	ATOM	223	0	TRP	В	239	-35.423	63.772	7.388	1.00 71.7	70 8
	ATOM	224	N	LYS			-34.165	62.791	8.955	1.00 67.3	LO 7
	ATOM	225	CA	LYS			-33.724	61.744	8.077	1.00 65.0	63
	ATOM	226	CB	LYS			-33.321	60.539	8.906	1.00 66.0	55 6
5	5 ATOM	227	CG			240	-32.210	60.824	9.905	1.00 69.8	33 6
	ATOM	228	CD	LYS				59.553	10.602	1.00 71.4	
	ATOM	229	CE	LYS				59.843	11.493	1.00 71.3	
	ATOM	230	NZ			240		58.604	12.157	1.00 72.2	
	ALOM	230	1477	טובט	٠	_ 10	55.100	,			

	5	ATOM	231	С	LYS	В	240	-34.719	61.331	6.996		66.19	6
		ATOM	232	0	LYS	В	240	-34.321	60.673	6.031	1.00	65.20	8
		ATOM	233	N	ASN	В	241	-35.986	61.727	7.139		66.69	7
		ATOM	234	CA	ASN	В	241	-37.031	61.393	6.171		67.53	6
		ATOM	235	CB	ASN	В	241	-38.240	60.846	6.915		67.98	6
	10	ATOM	236	CG	ASN	В	241	-37.966	59.479	7.544	1.00	70.19	6
		ATOM	237	OD1	ASN	В	241	-37.561	58.526	6.845	1.00	71.37	8
		ATOM	238	ND2	ASN	В	241	-38.205	59.370	8.836	1.00	71.48	7
		ATOM	239	С	ASN	В	241	-37.496	62.532	5.255	1.00	66.62	6
		ATOM	240	0	ASN	В	241	-38.504	62.395	4.578	1.00	64.76	8
	15	ATOM	241	N	LYS	В	242	-36.753	63.633	5.209	1.00	66.86	7
		ATOM	242	CA	LYS	В	242	-37.096	64.772	4.362	1.00	67.46	6
		ATOM	243	CB	LYS		242	-37.501	65.948	5.258	1.00	67.93	6
		ATOM	244	CG	LYS	В	242	-38.746	65.684	6.076	1.00	71.52	6
		ATOM	245	CD	LYS	В	242	-40.007	65.528	5.215	1.00	74.32	6
	20	ATOM	246	CE	LYS	В	242	-40.416	66.852	4.564	1.00	74.41	6
		ATOM	247	NZ	LYS	В	242	-40.657	67.941	5.575	1.00	74.44	7
		ATOM	248	С	LYS	В	242	-35.826	65.081	3.592	1.00	66.28	6
		ATOM	249	0	LYS	В	242	-35.814	65.799	2.601	1.00	67.61	8
(11)		ATOM	250	N	ARG	В	243	-34.763	64.485	4.112	1.00	64.19	7
10	25	ATOM	251	CA	ARG	В	243	-33.410	64.577	3.591	1.00	62.43	6
ľÚ		ATOM	252	CB	ARG	В	243	-32.599	63.547	4.390	1.00	60.12	6
(1)		ATOM	253	CG	ARG	В	243	-31.128	63.558	4.171	1.00	40.00	6
lut.		ATOM	254	CD	ARG	В	243	-30.335	62.888	5.319		40.00	6
N		ATOM	255	NE	ARG	В	243	-30.269	61.428	5.296		40.00	7
land.	30	ATOM	256	CZ	ARG	В	243	-29.384	60.724	6.009		40.00	6
14		ATOM	257	NH1	ARG	В	243	-28.510	61.357	6.798		40.00	7
10 (100)		MOTA	258	NH2	ARG	В	243	-29.355	59.401	5.908		40.00	7
		ATOM	259	С	ARG	В	243	-33.408	64.252	2.100		62.97	6
		ATOM	260	0	ARG	В	243	-33.690	63.122	1.722		63.96	8
BAS STATE	35	ATOM	261	N	LYS			-33.105	65.245	1.270		62.41	7
SECE		ATOM	262	CA	LYS			-33.054	65.053	-0.179		61.57	6
. 71		ATOM	263	CB	LYS			-34.104	65.941	-0.866		63.68	6
22.7		ATOM	264	CG	LYS			-35.527	65.731	-0.337		71.29	6
		ATOM	265	CD	LYS			-36.566	66.549	-1.107		73.83	6
	40	ATOM	266	CE	LYS			-36.219	68.045	-1.138		74.71	6
		ATOM	267	ΝZ	LYS			-36.169	68.689	0.219		73.32	7
		ATOM	268	С	LYS			-31.658	65.402	-0.670		59.30	6 8
		ATOM	269	0	LYS			-31.317	66.570	-0.852		56.34	7
		ATOM	270	N	PHE		245	-30.858	64.359	-0.875		57.06	6
	45	ATOM	271	CA			245	-29.462	64.525	-1.305		59.01	6
		ATOM	272	CB			245	-28.786	63.179	-1.478		59.62	
		ATOM	273	CG			245	-28.991	62.288	-0.339		66.60	6 6
		ATOM	274		PHE		245	-30.200	61.669	-0.172		67.17 69.25	6
		ATOM	275	CD2				-28.012	62.117	0.593		69.92	6
	50	ATOM	276	CE1				-30.404	60.882	0.911 1.669		70.50	6
		ATOM	277	CE2			245	-28.229	61.329	1.830		70.89	6
		ATOM	278	CZ			245	-29.418	60.714			60.68	6
		ATOM	279	С			245	-29.301	65.282	-2.592		62.37	8
		ATOM	280	0			245	-29.859	64.911 66.336	-3.619 -2.505		60.10	7
	55	ATOM	281	N			246 246	-28.495 -28.201	67.199	-3.631		59.44	6
		ATOM	282	CA CB			246	-27.248	68.332	-3.231		57.43	6
		ATOM	283	CB			246	-27.240	69.474	-4.207		54.41	6
		ATOM	284	CG	The C	D	240	21.110	55 3	1.20,			-

	5	ATOM	101	CA	LYS	В	274	-31.983	79.774	-2.147	1.00	54.53	6
		ATOM	102	CB	LYS	В	274	-32.133	78.724	-3.232	1.00	54.36	6
		ATOM	103	С	LYS		274	-32.819	79.396	-0.931	1.00	56.88	6
		ATOM	104	0	LYS		274	-34.025	79.624	-0.906	1.00	57.98	8
		ATOM	105	N	ILE		275	-32.151	78.820	0.076	1.00	56.48	7
	10	ATOM	106	CA	ILE		275	-32.791	78.381	1.332	1.00	52.64	6
	10	ATOM	107	CB	ILE		275	-32.638	76.863	1.519	1.00		6
		ATOM	108	CG2	ILE		275	-33.505	76.105	0.529	1.00		6
		ATOM	100	CG1	ILE		275	-31.188	76.441	1.343	1.00		6
				CD1	ILE		275	-30.990	74.952	1.391	1.00		6
	1.5	ATOM	110					-32.241	79.086	2.574	1.00		6
	15	ATOM	111	C	ILE		275	-32.858	79.049	3.622	1.00		8
		ATOM	112	0	ILE				79.709	2.435		51.76	7
		ATOM	113	N	ILE		276	-31.071		3.533	1.00		6
		ATOM	114	CA	ILE		276	-30.410	80.409			55.04	6
		ATOM	115	CB	ILE		276	-29.145	81.110	3.042			
	20	ATOM	116	CG2	ILE		276	-29.486	82.172	2.017		53.28	6
		ATOM	117	CG1	ILE		276	-28.396	81.786	4.203	1.00		6
		MOTA	118	CD1	ILE			-27.862	80.854	5.231		60.32	6
		MOTA	119	С	ILE		276	-31.282	81.461	4.237		50.70	6
		ATOM	120	0	ILE		276	-31.015	81.817	5.385		55.55	8
153	25	ATOM	121	N	THR		277	-32.322	81.953	3.568		47.33	7
174		MOTA	122	CA	THR		277	-33.174	82.968	4.141		42.59	6
100		MOTA	123	CB	THR	В	277	-34.042	83.632	3.048		44.97	6
- deng		ATOM	124	OG1	THR		277	-33.202	84.145	2.001		46.38	8
N		ATOM	125	CG2	THR	В	277	-34.856	84.781	3.653		37.17	6
fash	30	ATOM	126	С	THR		277	-34.069	82.447	5.267		39.84	6
1		MOTA	127	0	THR	В	277	-34.083	83.026	6.375		40.55	8
#1		ATOM	128	N	PRO	В	278	-34.832	81.385	5.017		38.20	7
100		ATOM	129	CD	PRO	В	278	-34.925	80.666	3.747		36.34	6
i.i		ATOM	130	CA	PRO	В	278	-35.711	80.834	6.059		36.63	6
W	35	ATOM	131	CB	PRO	В	278	-36.475	79.715	5.357		32.95	6
U		ATOM	132	CG	PRO	В	278	-35.833	79.516	4.056		35.75	6
100		ATOM	133	C	PRO	В	278	-34.892	80.324	7.220		38.60	6
127		ATOM	134	0	PRO	В	278	-35.372	80.157	8.331		37.67	8
		ATOM	135	N	ALA	В	279	-33.636	80.040	6.927	1.00	37.05	7
	40	ATOM	136	CA	ALA	В	279	-32.696	79.525	7.903	1.00	33.18	6
		MOTA	137	CB	ALA	В	279	-31.391	79.195	7.205	1.00	30.56	6
		MOTA	138	С	ALA	В	279	-32.447	80.536	8.991	1.00	33.47	6
		ATOM	139	0	ALA	В	279	-32.623	80.238	10.158	1.00	33.74	8
		ATOM	140	N	ILE	В	280	-32.010	81.728	8.577	1.00	29.96	7
	45	ATOM	141	CA	ILE	В	280	-31.728	82.809	9.501	1.00	25.94	6
		ATOM	142	CB	ILE	В	280	-31.190	84.040	8.754	1.00	26.95	6
		ATOM	143	CG2	ILE			-30.881	85.149	9.715	1.00	15.40	6
		ATOM	144	CG1				-29.904	83.696	8.007	1.00	26.73	6
		ATOM	145		ILE			-29.255	84.878	7.362	1.00	34.31	6
	50	ATOM	146	C	ILE				83.172	10.310	1.00	31.39	6
	50	ATOM	147	o	ILE				83.378	11.522		35.69	8
		ATOM	148	N	THR		281	-34.113	83.233	9.647		30.90	7
		ATOM	149	CA	THR		281	-35.361	83.586	10.328		33.49	6
				CB	THR		281		83.396	9.419		37.18	6
	55	ATOM	150	OG1				-36.703	82.034	9.005		46.48	8
	33	ATOM	151 152	CG2					84.289	8.198		32.85	6
		ATOM					281		82.706	11.556		29.94	6
		ATOM	153	C				-35.855	83.186	12.634		25.55	8
		ATOM	154	0	THE	B	281	-33.633	00.100	12.034	1.00	~ ~ . ~ ~ ~	0

	5	ATOM	263	CA	GLU	В	295	-34.839	92.159	27.816	1.00	52.53	6
		ATOM	264	CB	GLU	В	295	-34.553	91.412	29.131	1.00	57.40	6
		ATOM	265	CG	GLU	В	295	-35.811	90.978	29.874	1.00	69.63	6
		ATOM	266	CD	GLU	В	295	-36.610	92.144	30.375	1.00	78.49	6
		ATOM	267	OE1	GLU	В	295	-36.153	92.869	31.297	1.00	82.82	8
	10	ATOM	268		GLU		295	-37.730	92.385	29.860	1.00	85.30	8
	10	ATOM	269	C	GLU			-33.629	93.009	27.415	1.00	48.54	6
		ATOM	270	0	GLU		295	-32.981	93.627	28.260	1.00	49.82	8
		ATOM	271	N	LEU		296	-33.374	93.030	26.109		43.79	7
		ATOM	272	CA	LEU		296	-32.268	93.761	25.540	1.00	45.42	6
	15	ATOM	273	CB	LEU		296	-31.319	92.769	24.838		41.04	6
	15	ATOM	274	CG	LEU			-30.735	91.631	25.662		42.74	6
		ATOM	275		LEU		296	-30.354	90.478	24.764		40.99	6
		ATOM	276		LEU		296	-29.559	92.119	26.468		39.44	6
		ATOM	277	C	LEU		296	-32.760	94.779	24.522		45.56	6
	20		278	0	LEU		296	-33.845	94.600	23.924		43.07	8
	20	ATOM			PRO		297	-32.004	95.875	24.338		46.99	7
		ATOM	279	И			297	-30.740	96.123	25.046		47.12	6
		ATOM	280	CD	PRO				96.123	23.363		49.61	6
1222		ATOM	281	CA	PRO PRO		297	-32.388 -31.294	97.973	23.494		49.91	6
1,5	0.5	ATOM	282	CB				-30.302	97.477	24.545		51.28	6
10	25	ATOM	283	CG	PRO				96.273	21.913		49.59	6
111		ATOM	284	С	PRO		297	-32.263				51.66	8
170 July		ATOM	285	0	PRO		297	-31.441	95.340	21.685		51.00	7
14		ATOM	286	N	CYS		298	-33.035	96.667	20.854		52.86	6
li-é		ATOM	287	CA	CYS			-32.761	96.150	19.456			6
143	30	MOTA	288	CB	CYS			-33.140	97.165	18.356		54.57	16
11		ATOM	289	SG	CYS			-34.884	97.085	17.836		67.87 48.51	6
ind tred		ATOM	290	С	CYS			-31.385	96.330	19.127		49.58	8
[1]		ATOM	291	0	CYS			-30.579	95.506	18.744			7
		ATOM	292	N	GLU			-31.107	97.447	19.230		44.17	6
10	35	ATOM	293	CA	GLU		299	-29.989	97.645	18.718		47.57	
ıĎ.		ATOM	294	CB	GLU		299	-29.402	98.973	19.208		49.92	6
4D		ATOM	295	CG			299	-29.944		18.433		59.30	6
120		MOTA	296	CD	GLU		299	-31.090		19.164		63.80	6
		MOTA	297		GLU					18.629		69.03	8
	40	ATOM	298		GLU					20.319		67.10	8
		MOTA	299	С			299		96.533	18.987		46.57	6
		ATOM	300	0			299		96.179	18.111		44.65	8
		ATOM	301	N			300	-29.045	95.989	20.203		45.17	7
		ATOM	302	CA			300	-28.152	94.908	20.584		43.32	6
	45	ATOM	303	CB	ASP		300	-27.985	94.849	22.105		37.38	6
		ATOM	304	CG	ASP	В	300		96.016	22.650		36.23	6
		ATOM	305	OD1	ASP	В	300	-26.208	96.421	22.052		35.87	8
		ATOM	306	OD2	ASP		300		96.543	23.716		40.14	8
		ATOM	307	С	ASP	В	300		93.591	20.071		42.81	6
	50	ATOM	308	0	ASP	В	300	-28.001	92.775	19.489		46.02	8
		ATOM	309	N	GLN	В	301	-30.019	93.399	20.306		38.60	7
		ATOM	310	CA	GLN	В	301		92.197	19.858		40.00	6
		ATOM	311	CB	GLN	В	301	-32.234	92.418	19.836		38.59	6
		ATOM	312	CG	GLN	В	301	-32.908	92.380	21.187		40.26	6
	55	ATOM	313	CD	GLN	В	301	-34.401	92.583	21.083		44.15	6
		ATOM	314	OE1	GLN	В	301	-34.859	93.637	20.589		45.73	8
		ATOM	315	NE2	GLN	В	301	-35.165	91.602	21.544		46.13	7
		ATOM	316	С	GLN	В	301	-30.237	91.830	18.455	1.00	41.64	6

	5	ATOM	317	0	GLN	В	301	-30.162	90.662	18.100	1.00	45.02	8
		ATOM	318	N	ILE	В	302	-29.916	92.864	17.674	1.00	41.01	7
		ATOM	319	CA	ILE	В	302	-29.424	92.692	16.311	1.00	40.23	6
		ATOM	320	CB	ILE	В	302	-29.584	93.978	15.498	1.00	39.52	6
		ATOM	321	CG2	ILE	В	302	-29.034	93.792	14.100	1.00	31.98	6
	10		322	CG1	ILE	В	302	-31.059	94.385	15.416	1.00	40.77	6
		ATOM	323	CD1	ILE	В	302	-31.939	93.317	14.775	1.00	45.43	6
		ATOM	324	С	ILE	В	302	-27.966	92.260	16.342	1.00	38.58	6
		ATOM	325	0	ILE	В	302	-27.613	91.197	15.830	1.00	40.81	8
		ATOM	326	N	ILE	В	303	-27.128	93.111	16.933	1.00	37.50	7
	15		327	CA	ILE	В	303	-25.692	92.846	17.062	1.00	39.33	6
		ATOM	328	CB	ILE	В	303	-25.066	93.648	18.203	1.00	39.06	6
		MOTA	329	CG2	ILE	В	303	-23.566	93.405	18.257	1.00	36.19	6
		ATOM	330	CG1	ILE	В	303	-25.309	95.143	18.020	1.00	40.15	6
		ATOM	331	CD1	ILE	В	303	-24.816	95.966	19.173	1.00	36.93	6
	20		332	С	ILE	В	303	-25.470	91.365	17.323	1.00	36.49	6
		ATOM	333	0	ILE	В	303	-24.619	90.725	16.712	1.00	36.58	8
		ATOM	334	N	LEU	В	304	-26.244	90.843	18.266	1.00	32.91	7
		ATOM	335	CA	LEU	В	304	-26.194	89.433	18.633	1.00	27.55	6
1	3	ATOM	336	CB	LEU	В	304	-27.172	89.182	19.793	1.00	22.35	6
5	5 25	ATOM	337	CG	LEU	В	304	-26.623	89.449	21.187	1.00	26.88	6
	1	ATOM	338	CD1	LEU	В	304	-25.540	90.495	21.136		24.82	6
1	1	ATOM	339	CD2	LEU	В	304	-27.747	89.840	22.121	1.00	23.69	6
	di-	ATOM	340	C	LEU	В	304	-26.505	88.547	17.425	1.00	28.05	6
	ų.	ATOM	341	0	LEU	В	304	-25.668	87.751	16.983		24.68	8
60		MOTA	342	N	LEU	В	305	-27.716	88.700	16.897		26.34	7
	ni Jo	ATOM	343	CA	LEU		305	-28.145	87.939	15.741		30.91	6
81	ring.	MOTA	344	CB	LEU	В	305	-29.460	88.514	15.199		32.50	6
-	The same	ATOM	345	CG	LEU		305	-30.699	88.305	16.050		33.36	6
9	, i	MOTA	346		LEU		305	-31.938	88.839	15.342		33.87	6
90	35	MOTA	347	CD2	LEU		305	-30.863	86.812	16.298		31.72	6
13	d O	ATOM	348	C	LEU		305	-27.072	87.922	14.666		29.76	6
	Ó	MOTA	349	0	LEU			-26.687	86.860	14.202		29.33	8
	92	MOTA	350	N	LYS		306	-26.597	89.107	14.291		29.72	7
		MOTA	351	CA	LYS		306	-25.576	89.254	13.264		34.28	6
	40		352	CB	LYS		306	-25.224	90.732	13.077		35.98	6
		MOTA	353	CG	LYS		306	-26.350	91.581	12.494		43.35	6
		ATOM	354	CD	LYS		306	-25.852	92.987	12.182		51.50	6 6
		ATOM	355	CE	LYS		306	-24.706	92.932	11.190		53.26	7
		ATOM	356	NZ	LYS		306	-23.883	94.161	11.251		59.61	6
	45		357	С	LYS		306	-24.308	88.484	13.556		35.25	8
		ATOM	358	0		В	306	-23.681	87.917	12.653		33.95	7
		ATOM	359	N	GLY		307	-23.918	88.478	14.829		35.79 34.59	6
		ATOM	360	CA			307	-22.702	87.793	15.227		33.80	6
		ATOM	361	С	GLY		307	-22.811	86.291	15.383		31.59	8
	50		362	0	GLY			-21.944	85.564	14.895		31.15	7
		ATOM	363	N	CYS		308	-23.861	85.843	16.071		29.04	6
		ATOM	364	CA			308	-24.069	84.434	16.320 17.663		27.59	6
		ATOM	365	CB			308	-24.761	84.240			30.50	16
	۰.,	ATOM	366	SG				-26.496	84.629 83.712	17.608 15.266		30.59	6
	55		367	С	CYS			-24.911 -25.088	82.499	15.365		33.77	8
		ATOM	368	0	CYS			-25.432	84.429	14.266		28.46	7
		ATOM	369	N				-25.432 -26.270	83.787	13.265		30.10	6
		ATOM	370	CA	CYS	D	309	-20.270	00.101	10.200	1.00	50.10	_

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	-	3 moss	522	0	THR	ъ	220	-29.432	69.801	7.535	1 00	43.72	8
	5	ATOM	533					-28.589	70.413	5.546		44.62	7
		ATOM	534	N	LEU				71.812	5.658		45.09	6
		ATOM	535	CA	LEU		330	-28.983					
		ATOM	536	CB	LEU			-28.354	72.608	4.510		44.66	6
		MOTA	537	CG	LEU		330	-26.847	72.735	4.539		51.06	6
	10	ATOM	538	CD1	LEU	В	330	-26.226	71.367	4.640		48.58	6
		ATOM	539	CD2	LEU	В	330	-26.364	73.450	3.299		45.18	6
		ATOM	540	С	LEU	В	330	-30.508	71.965	5.652		48.06	6
		ATOM	541	0	LEU	В	330	-31.211	71.244	4.959	1.00	49.33	8
		ATOM	542	N	ASN	В	331	-30.988	72.911	6.458	1.00	52.20	7
	15	ATOM	543	CA	ASN		331	-32.407	73.214	6.588	1.00	54.41	6
		ATOM	544	СВ	ASN		331	-32.870	74.013	5.370	1.00	54.94	6
		ATOM	545	CG	ASN		331	-33.687	75.220	5.749	1.00	60.35	6
		ATOM	546		ASN		331	-33.182	76.130	6.430	1.00	61.84	8
			547		ASN		331	-34.935	75.242	5.324		65.92	7
	20	ATOM			ASN		331	-33.251	71.959	6.731		58.00	6
	20	ATOM	548	C			331	-34.464	72.000	6.579		60.17	8
		ATOM	549	0	ASN			-32.596	70.846	7.054		58.45	7
		ATOM	550	N	GLY		332			7.034		58.55	6
		ATOM	551	CA	GLY		332	-33.295	69.587				6
100		ATOM	552	С	GLY		332	-33.909	69.004	5.984		59.79	8
·IQ	25	ATOM	553	0	GLY		332	-34.609	68.000	6.065		61.32	7
17,		ATOM	554	И	GLU		333	-33.639	69.628	4.838		60.28	
10		ATOM	555	CA	GLU		333	-34.196	69.182	3.571		59.13	6
10		ATOM	556	CB	GLU		333	-34.966	70.323	2.885		62.40	6
M		ATOM	557	CG	GLU		333	-36.099	70.963	3.690		75.69	6
fail.	30	ATOM	558	CD	GLU	В	333	-36.720	72.135	2.998		80.41	6
1.5		ATOM	559	OE1	GLU	В	333	-35.984	73.081	2.618		79.98	8
2(ATOM	560	OE2	GLU	В	333	-37.966	72.158	2.830		83.81	8
and a		MOTA	561	С	GLU	В	333	-33.110	68.722	2.624		57.18	6
Į.i		ATOM	562	0	GLU		333	-33.236	67.689	1.974		57.50	8
U	35	ATOM	563	N	MET	В	334	-32.054	69.528	2.539		55.20	7
1122		ATOM	564	CA	MET	В	334	-30.926	69.259	1.653		50.85	6
		ATOM	565	CB	MET	В	334	-30.514	70.563	0.984		48.70	6
10		ATOM	566	CG	MET	В	334	-29.244	70.460	0.194		45.39	6
		ATOM	567	SD	MET	В	334	-28.743	72.008	-0.624		44.56	16
	40	ATOM	568	CE	MET	В	334	-30.307	72.445	-1.503	1.00	45.25	6
		ATOM	569	С	MET	В	334	-29.711	68.634	2.319	1.00	51.59	6
		ATOM	570	0	MET	В	334	-29.185	69.161	3.291	1.00	52.52	8
		ATOM	571	N	ALA		335	-29.270	67.515	1.758	1.00	51.00	7
		ATOM	572	CA	ALA			-28.106	66.802	2.267	1.00	48.98	6
	45	ATOM	573	CB	ALA		335	-28.377	65.304	2.274	1.00	47.86	6
	43	ATOM	574	C	ALA		335	-26.931	67.108	1.371	1.00	51.01	6
		ATOM	575	0	ALA		335	-26.936	66.760	0.190		51.61	8
			576	N	VAL		336	-25.921	67.770	1.930		46.62	7
		ATOM		CA	VAL		336	-24.730	68.142	1.152		42.35	6
	50	ATOM	577				336	-24.466	69.635	1.258		42.41	6
	50	ATOM	578	CB	VAL			-25.695	70.418	0.860		42.00	6
		ATOM	579		VAL		336	-24.018	70.418	2.642		40.32	6
		ATOM	580		VAL		336					45.33	6
		ATOM	581	С	VAL		336	-23.493	67.390 66.775	1.611 2.681		47.42	8
		ATOM	582	0	VAL		336	-23.464	67.478	0.781		41.60	7
	55	ATOM	583	N		В	337	-22.461		1.041		39.69	6
		ATOM	584	CA	THR		337	-21.172	66.818			41.35	6
		ATOM	585	CB	THR		337	-20.720	66.011	-0.173			8
		MOTA	586	OG1	THR	В	337	-20.273	66.887	-1.213	1.00	49.35	В

	5	ATOM	641	С	GLY	В	344	-19.867	77.636	-2.258	1.00 38.26	6
		ATOM	642	0	GLY	В	344	-20.715	78.501	-2.484	1.00 35.69	8
		ATOM	643	N	GLY	В	345	-18.724	77.871	-1.619	1.00 35.89	7
		ATOM	644	CA	GLY	В	345	-18.426	79.209	-1.159	1.00 34.00	6
		ATOM	645	C	GLY	В	345	-17.848	79.298	0.230	1.00 38.64	6
	10	ATOM	646	0	GLY	В	345	-17.216	80.303	0.573	1.00 38.14	8
		ATOM	647	N	LEU	В	346	-18.071	78.266	1.041	1.00 39.52	7
		ATOM	648	CA	LEU	В	346	-17.563	78.279	2.403	1.00 36.05	6
		ATOM	649	CB	LEU	В	346	-18.311	77.256	3.269	1.00 35.72	6
		ATOM	650	CG	LEU	В	346	-19.800	77.473	3.378	1.00 34.89	6
	15	ATOM	651	CD1	LEU	В	346	-20.322	76.678	4.554	1.00 44.09	6
		ATOM	652	CD2	LEU	В	346	-20.086	78.937	3.612	1.00 34.84	6
		ATOM	653	С	LEU	В	346	-16.079	78.018	2.445	1.00 33.52	6
		ATOM	654	0	LEU	В	346	-15.392	78.387	3.394	1.00 35.58	8
		ATOM	655	N	GLY	В	347	-15.586	77.388	1.385	1.00 30.47	7
	20	ATOM	656	CA	GLY	В	347	-14.174	77.078	1.305	1.00 33.01	6
		ATOM	657	С	GLY	В	347	-13.768	76.214	2.477	1.00 30.72	6
		ATOM	658	0	GLY	В	347	-14.433	75.243	2.808	1.00 30.89	8
		ATOM	659	N	VAL		348	-12.647	76.585	3.087	1.00 31.30	7
(2)		ATOM	660	CA	VAL		348	-12.097	75.867	4.227	1.00 31.27	6
10	25	ATOM	661	CB	VAL	В	348	-10.889	76.609	4.817	1.00 31.66	6
17.5		ATOM	662	CG1	VAL	В	348	-11.292	77.974	5.360	1.00 20.19	6
Ü		ATOM	663	CG2	VAL	В	348	-10.250	75.786	5.905	1.00 24.77	6
		ATOM	664	С	VAL		348	-13.136	75.651	5.360	1.00 33.84	6
000		ATOM	665	ō	VAL		348	-13.002	74.707	6.153	1.00 29.99	8
g sale	30	ATOM	666	N	VAL	В	349	-14.157	76.518	5.449	1.00 33.31	7
150		ATOM	667	CA	VAL		349	-15.147	76.339	6.483	1.00 32.23	6
10		ATOM	668	СВ	VAL	В	349	-16.226	77.393	6.476	1.00 32.59	6
5027		ATOM	669	CG1	VAL	В	349	-17.342	76.979	7.399	1.00 33.68	6
1,4		ATOM	670		VAL	В	349	-15.667	78.703	6.959	1.00 32.30	6
IJ IJ	35	ATOM	671	С	VAL	В	349	-15.792	74.987	6.380	1.00 34.91	6
12		ATOM	672	0	VAL	В	349	-16.055	74.359	7.394	1.00 33.73	8
A.D.		ATOM	673	N	SER	В	350	-16.054	74.507	5.176	1.00 32.81	7
10		ATOM	674	CA	SER	В	350	-16.695	73.215	5.100	1.00 30.10	6
		ATOM	675	CB	SER	В	350	-16.772	72.697	3.684	1.00 24.95	6
	40	ATOM	676	OG	SER	В	350	-17.538	71.502	3.644	1.00 23.16	8
		ATOM	677	C	SER	В	350	-15.910	72.254	5.942	1.00 31.59	6
		ATOM	678	0	SER	В	350	-16.417	71.807	6.950	1.00 37.62	8
		ATOM	679	N	ASP	В	351	-14.675	71.942	5.565	1.00 28.60	7
		ATOM	680	CA	ASP	В	351	-13.905	71.010	6.378	1.00 29.82	6
	45	ATOM	681	CB	ASP	В	351	-12.419	71.139	6.050	1.00 27.49	6
		ATOM	682	CG	ASP	В	351	-12.151	71.094	4.585	1.00 30.22	6
		ATOM	683	OD1	ASP	В	351	-12.013	72.174	3.954	1.00 32.61	8
		ATOM	684	OD2	ASP	В	351	-12.064	69.980	4.017	1.00 30.02	8
		ATOM	685	C	ASP	В	351	-14.176	71.343	7.861	1.00 30.63	6
	50	ATOM	686	0	ASP	В	351	-14.458	70.474	8.681	1.00 29.54	8
		ATOM	687	N	ALA	В	352	-14.111	72.629	8.177	1.00 25.33	7
		ATOM	688	CA	ALA	В	352	-14.346	73.092	9.533	1.00 28.59	6
		ATOM	689	CB	ALA	В	352	-14.252	74.606	9.572	1.00 20.95	6
		ATOM	690	C	ALA	В	352	-15.690	72.630	10.086	1.00 29.69	6
	55	ATOM	691	0	ALA	В	352	-15.757	72.068	11.164	1.00 30.36	8
		ATOM	692	N	ILE	В	353	-16.754	72.884	9.330	1.00 27.63	7
		ATOM	693	CA	ILE	В	353	-18.096	72.506	9.729	1.00 27.55	6
		ATOM	694	CB	ILE	В	353	-19.144	73.129	8.800	1.00 28.04	6

	5	ATOM	695	CG2	ILE	В	353	-20.529	72.673	9.195	1.00 23.68	
		ATOM	696	CG1	ILE	В	353	-19.108	74.657	8.869	1.00 27.33	6
		ATOM	697	CD1	ILE	В	353	-20.141	75.313	7.964	1.00 26.23	6
		ATOM	698	С	ILE	В	353	-18.309	71.002	9.775	1.00 30.88	6
		ATOM	699	ō	ILE		353	-19.021	70.499	10.639	1.00 31.22	
	10	ATOM	700	N	PHE		354	-17.728	70.279	8.822	1.00 29.86	
	10				PHE			-17.881	68.831	8.797	1.00 31.08	
		ATOM	701	CA						7.439	1.00 28.80	
		ATOM	702	CB			354	-17.461	68.249			
		ATOM	703	CG	PHE		354	-18.568	68.233	6.405	1.00 28.80	
		ATOM	704		PHE			-19.031	69.403	5.833	1.00 30.96	
	15	ATOM	705	CD2	PHE		354	-19.150	67.027	6.034	1.00 29.45	
		ATOM	706	CE1	PHE	В	354	-20.066	69.362	4.902	1.00 27.12	
		ATOM	707	CE2	PHE	В	354	-20.186	66.978	5.104	1.00 25.19	
		ATOM	708	CZ	PHE	В	354	-20.644	68.146	4.535	1.00 28.09	6
		ATOM	709	С	PHE	В	354	-17.041	68.223	9.913	1.00 29.17	6
	20	ATOM	710	0	PHE			-17.544	67.429	10.700	1.00 32.62	8
		ATOM	711	N	ASP		355	-15.761	68.593	9.972	1.00 23.86	7
		ATOM	712	CA	ASP			-14.864	68.090	11.005	1.00 25.34	6
		ATOM	713	CB	ASP		355	-13.582	68.929	11.045	1.00 21.41	
7:26			714	CG	ASP		355	-12.548	68.456	10.086	1.00 32.08	
	25	ATOM						-12.899	68.069	8.944	1.00 32.00	
100	25	ATOM	715		ASP						1.00 33.30	
113		ATOM	716		ASP			-11.345	68.477	10.450		
10		ATOM	717	С	ASP			-15.570	68.153	12.357	1.00 27.86	
j-k		MOTA	718	0	ASP		355	-15.430	67.257	13.182	1.00 32.42	
-		ATOM	719	N	LEU			-16.339	69.223	12.561	1.00 26.84	
100	30	MOTA	720	CA	LEU		356	-17.085	69.400	13.803	1.00 28.66	
11		ATOM	721	CB	LEU	В	356	-17.832	70.742	13.800	1.00 25.37	
23		MOTA	722	CG	LEU	В	356	-18.655	71.091	15.023	1.00 27.61	. 6
(.)		ATOM	723	CD1	LEU	В	356	-17.729	71.248	16.191	1.00 25.43	6
14		ATOM	724	CD2	LEU	В	356	-19.430	72.363	14.808	1.00 27.49	6
	35	ATOM	725	С	LEU		356	-18.084	68.260	13.883	1.00 30.44	6
1200	55	ATOM	726	0			356	-18.054	67.445	14.804	1.00 31.55	
+0		ATOM	727	N			357	-18.972	68.214	12.891	1.00 32.69	7
12		ATOM	728	CA			357	-20.001	67.186	12.846	1.00 29.87	
			729	C			357	-19.486	65.832	13.279	1.00 33.12	
	40	ATOM					357	-20.032	65.246	14.207	1.00 29.41	
	40	ATOM	730	0				-18.444	65.351	12.593	1.00 23.41	
		MOTA	731	N			358				1.00 35.87	
		MOTA	732	CA			358	-17.834	64.066	12.902		
		MOTA	733	CB			358	-16.513	63.903	12.151	1.00 34.56	
		MOTA	734	CG			358	-16.649	63.908	10.657	1.00 46.43	
	45	MOTA	735	SD			358	-15.094	63.597	9.751	1.00 42.13	
		MOTA	736	CE			358	-14.121	65.063	10.228	1.00 44.29	
		MOTA	737	С	MET	В	358	-17.552	63.976	14.392	1.00 33.26	
		ATOM	738	0	MET	В	358	~18.019	63.075	15.075	1.00 36.39	8
		ATOM	739	N	SER	В	359	-16.766	64.933	14.875	1.00 33.31	. 7
	50	ATOM	740	CA	SER	В	359	-16.380	64.998	16.270	1.00 34.39	6
	50	ATOM	741	CB			359	-15.724	66.339	16.541	1.00 30.84	
		ATOM	742	OG			359	-15.130	66.355	17.825	1.00 47.14	
		ATOM	743	C	SER			-17.579	64.813	17.169	1.00 36.43	
							359	-17.635	63.853	17.922	1.00 35.46	
		ATOM	744	0				-18.525	65.744	17.079	1.00 36.74	
	55	MOTA	745	N	LEU						1.00 35.44	
		ATOM	746	CA	LEU		360	-19.741	65.729	17.889	1.00 35.44	
		ATOM	747	CB	LEU			-20.706	66.817	17.405		
		ATOM	748	CG	LEU	В	360	-20.263	68.255	17.575	1.00 34.59	ט י

	5	MOTA	857	OE1	GLN	В	374	-29.720	75.049	18.009	1.00 24.07	8
		ATOM	858	NE2	GLN	В	374	-30.473	76.980	18.901	1.00 25.59	7
		ATOM	859	C	GLN	В	374	-26.988	79.249	21.569	1.00 20.66	6
		ATOM	860	0	GLN	В	374	-26.733	80.307	20.994	1.00 24.47	8
		ATOM	861	N	ALA	В	375	-27.429	79.182	22.825	1.00 16.26	7
	10	ATOM	862	CA	ALA	В	375	-27.639	80.374	23.631	1.00 17.16	6
		ATOM	863	CB	ALA	В	375	-28.435	80.025	24.865	1.00 19.53	6
		ATOM	864	С	ALA	В	375	-26.304	80.966	24.025	1.00 25.13	6
		ATOM	865	0	ALA	В	375	-26.074	82.154	23.833	1.00 23.81	8
		ATOM	866	N	VAL	В	376	-25.433	80.111	24.568	1.00 24.57	7
	15	ATOM	867	CA	VAL	В	376	-24.102	80.526	24.986	1.00 25.80	6
		ATOM	868	CB	VAL	В	376	-23.192	79.321	25.234	1.00 26.48	6
		ATOM	869	CG1	VAL	В	376	-21.806	79.780	25.620	1.00 23.20	6
		ATOM	870	CG2	VAL	В	376	-23.771	78.433	26.310	1.00 19.08	6
		ATOM	871	С	VAL	В	376	-23.510	81.403	23.898	1.00 25.69	6
	20	ATOM	872	0	VAL	В	376	-22.796	82.364	24.166	1.00 27.87	8
		ATOM	873	N	LEU	В	377	-23.827	81.049	22.659	1.00 23.09	7
		ATOM	874	CA	LEU	В	377	-23.340	81.774	21.492	1.00 22.86	6
		ATOM	875	CB	LEU	В	377	-23.552	80.920	20.230	1.00 18.50	6
(2)		ATOM	876	CG	LEU	В	377	-22.756	79.638	20.146	1.00 22.65	6
453	25	ATOM	877	CD1	LEU	В	377	-23.221	78.786	19.000	1.00 16.70	6
[7]		ATOM	878	CD2	LEU	В	377	-21.300	79.995	20.000	1.00 19.58	6
tio		ATOM	879	C	LEU	В	377	-24.073	83.102	21.384	1.00 26.14	6
1.3		ATOM	880	0	LEU	В	377	-23.464	84.164	21.419	1.00 20.62	8
1		ATOM	881	N	LEU	В	378	-25.396	83.023	21.265	1.00 28.99	7
g safe	30	ATOM	882	CA	LEU	В	378	-26.228	84.217	21.147	1.00 28.87	6
79.43		ATOM	883	CB	LEU	В	378	-27.696	83.894	21.450	1.00 26.89	6
81		ATOM	884	CG	LEU	В	378	-28.648	85.068	21.500	1.00 28.83	6
(3		ATOM	885	CD1	LEU	В	378	-28.507	85.854	20.225	1.00 27.97	6
I,t,		ATOM	886	CD2	LEU	В	378	-30.072	84.605	21.692	1.00 27.69	6
	35	ATOM	887	C	LEU	В	378	-25.738	85.280	22.090	1.00 31.09	6
First Line		MOTA	888	0	LEU	В	378	-25.398	86.379	21.651	1.00 31.77	8
10		ATOM	889	N	MET	В	379	-25.695	84.931	23.376	1.00 31.44	7
1555		MOTA	890	CA	MET	В	379	-25.291	85.851	24.434	1.00 32.62	6
		ATOM	891	CB	MET	В	379	-25.797	85.335	25.793	1.00 31.45	6
	40	ATOM	892	CG		В	379	-27.332	85.262	25.883	1.00 38.75	6
		ATOM	893	SD	MET	В	379	-28.020	86.915	25.550	1.00 41.27	16
		ATOM	894	CE	MET	В	379	-29.814	86.586	25.513	1.00 35.68	6
		ATOM	895	C	MET		379	-23.796	86.129	24.538	1.00 33.72	6
		ATOM	896	0		В	379	-23.246	86.190	25.633	1.00 36.29	8
	45	ATOM	897	N	SER		380	-23.152	86.335	23.399	1.00 34.49	7
		ATOM	898	CA	SER		380	-21.738	86.659	23.391	1.00 33.97	6
		ATOM	899	CB	SER		380	-21.132	86.360	22.010	1.00 31.24	6
		ATOM	900	OG	SER		380	-21.224	84.978	21.696	1.00 39.42	8
		ATOM	901	C	SER		380	-21.635	88.145	23.705	1.00 39.69	6
	50	ATOM	902	0	SER		380	-22.084	88.989	22.933	1.00 44.64	8
		ATOM	903	N	SER		381	-21.053	88.451	24.857	1.00 41.04	7
		ATOM	904	CA	SER		381	-20.907	89.826	25.308	1.00 44.91	6
		ATOM	905	CB	SER		381	-20.610	89.832	26.797	1.00 44.50	6
		ATOM	906	OG	SER		381	-19.351	89.229	27.037	1.00 45.42	8
	55	ATOM	907	С	SER		381	-19.815	90.614	24.602	1.00 44.59	6
		ATOM	908	0	SER		381	-19.725	91.825	24.751	1.00 49.32	8
		ATOM	909	N	ASP		382	-18.977	89.922	23.848	1.00 43.75	7
		ATOM	910	CA	ASP	В	382	-17.886	90.556	23.144	1.00 43.93	6

	5	ATOM	1073	CG	PHE	В	403	-24.557	73.908	28.359	1.00 26	5.97	6
		ATOM	1074	CD1	PHE	В	403	-23.916	74.494	27.272	1.00 25	5.55	6
		ATOM	1075	CD2	PHE	В	403	-24.939	72.583	28.271	1.00 19	9.75	6
		ATOM	1076	CE1	PHE	В	403	-23.670	73.765	26.104	1.00 27	7.90	6
		ATOM	1077	CE2	PHE		403	-24.693	71.848	27.102	1.00 22	2.56	6
	10	ATOM	1078	CZ			403	-24.057	72.439	26.020	1.00 22	2.24	6
		ATOM	1079	C	PHE		403	-24.810	72.902	31.329	1.00 28		6
		ATOM	1080	Ö	PHE		403	-25.092	71.726	31.205	1.00 20		8
					GLU		404	-23.776	73.335	32.037	1.00 30		7
		ATOM	1081	N					72.419	32.712	1.00 34		6
		ATOM	1082	CA	GLU		404	-22.865					
	15	ATOM	1083	CB	GLU		404	-21.835	73.215	33.527	1.00 39		6
		ATOM	1084	CG	GLU		404	-20.654	72.384	34.068	1.00 4		6
		ATOM	1085	CD	GLU		404	-19.750	73.129	34.996	1.00 5		6
		ATOM	1086	OE1	GLU	В	404	-19.372	74.290	34.701	1.00 5		8
		ATOM	1087	OE2	GLU	В	404	-19.369	72.555	36.048	1.00 63		8
	20	ATOM	1088	С	GLU	В	404	-23.645	71.509	33.642	1.00 3		6
		ATOM	1089	0	GLU	В	404	-23.470	70.292	33.640	1.00 38	8.64	8
		ATOM	1090	N	HIS	В	405	-24.492	72.131	34.458	1.00 29	9.56	7
		ATOM	1091	CA	HIS	В	405	-25.306	71.387	35.405	1.00 3	1.69	6
(3		ATOM	1092	CB	HIS	В	405	-26.245	72.324	36.173	1.00 33	3.75	6
A TO	25	ATOM	1093	CG	HIS		405	-25.536	73.185	37.163	1.00 3	4.75	6
TU	20	ATOM	1094		HIS		405	-24.234	73.286	37.524	1.00 3		6
CO		ATOM	1095		HIS		405	-26.223	74.101	37.969	1.00 3		7
luk.		ATOM	1096		HIS		405	-25.334	74.703	38.769	1.00 3		6
half			1090		HIS		405	-24.139	74.222	38.511	1.00 3		7
1.4	20	ATOM			HIS		405	-26.106	70.342	34.648	1.00 3		6
1	30	ATOM	1098	C					69.160	35.006	1.00 3		8
10		ATOM	1099	0	HIS			-26.087		33.598	1.00 3		7
(2)		ATOM	1100	N	TYR			-26.806	70.776	32.796	1.00 3		6
1,1,5		ATOM	1101	CA	TYR		406	-27.592	69.853				
		ATOM	1102	CB	TYR		406	-28.192	70.537	31.579	1.00 3		6
	35	ATOM	1103	CG	TYR		406	-28.991	69.576	30.730	1.00 2		6
100		ATOM	1104		TYR		406	-30.179	69.047	31.196	1.00 1		6
150		ATOM	1105	CE1			406	-30.893	68.128	30.441	1.00 2		6
549		MOTA	1106	CD2	TYR	В	406	-28.525	69.152	29.496	1.00 2		6
		ATOM	1107	CE2	TYR	В	406	-29.241	68.228	28.740	1.00 2		6
	40	ATOM	1108	CZ	TYR	В	406	-30.420	67.713	29.217	1.00 2		6
		ATOM	1109	OH	TYR	В	406	-31.120	66.802	28.480	1.00 2		8
		ATOM	1110	С	TYR	В	406	-26.697	68.725	32.304	1.00 2	4.24	6
		ATOM	1111	0	TYR	В	406	-27.155	67.609	32.110	1.00 2	7.08	8
		ATOM	1112	N	ILE	В	407	-25.422	69.056	32.084	1.00 2	5.76	7
	45	ATOM	1113	CA	ILE	В	407	-24.428	68.092	31.628	1.00 3	3.75	6
		ATOM	1114	CB	ILE	В	407	-23.090	68.778	31.274	1.00 3	4.23	6
		ATOM	1115		ILE		407	-21.959	67.774	31.230	1.00 3	2.46	6
		ATOM	1116	CG1			407	-23.214	69.514	29.936	1.00 4		6
		ATOM	1117	CD1			407	-23.655	68.612	28.804	1.00 4		6
	50	ATOM	1118	C	ILE		407	-24.191	67.004	32.658	1.00 3		6
	30						407	-24.178	65.806	32.343	1.00 3		8
		ATOM	1119	0					67.425	33.894	1.00 3		7
		ATOM	1120	N			408	-23.990					6
		ATOM	1121	CA	ASN	В	408	-23.739	66.475	34.943	1.00 3		
		ATOM	1122	CB	ASN		408	-23.524	67.221	36.256	1.00 3:		6
	55	ATOM	1123	CG	ASN	В	408	-22.296	68.137	36.202	1.00 3		6
		ATOM	1124		ASN	В	408	-21.194	67.696	35.823	1.00 3		8
		ATOM	1125		ASN		408	-22.478	69.397	36.604	1.00 3		7
		ATOM	1126	С	ASN	В	408	-24.876	65.453	35.036	1.00 3	8.14	6

	5	ATOM	1127	0	ASN	В	408	-24.624	64.25	3 35.105	1.00	42.16	8
		ATOM	1128	N	TYR			-26.122			1.00	35.62	7
		ATOM	1129	CA	TYR			-27.273				35.91	6
		ATOM	1130	CB	TYR		409	-28.597				34.41	6
		ATOM	1131	CG	TYR			-29.788				38.73	6
	10	ATOM	1132	CD1	TYR		409	-30.064				41.34	6
	10			CE1	TYR			-31.130				47.16	6
		ATOM	1133					-30.613				46.20	6
		ATOM	1134	CD2	TYR		409	-31.684				50.74	6
		ATOM	1135	CE2								50.88	6
	1.5	ATOM	1136	CZ	TYR			-31.942					8
	15	ATOM	1137	OH	TYR			-33.002				53.14 38.16	6
		ATOM	1138	С	TYR			-27.215				41.83	8
		ATOM	1139	0	TYR		409	-27.558					7
		ATOM	1140	N	ARG		410	-26.824				42.25	
		ATOM	1141	CA	ARG		410	-26.734				42.83	6
	20	ATOM	1142	CB	ARG		410	-26.350				36.83	6
		ATOM	1143	CG	ARG		410	-27.440				34.32	6
		ATOM	1144	CD	ARG		410	-28.284				36.62	6
		ATOM	1145	NE	ARG		410	-27.455				38.64	7
(say		ATOM	1146	CZ	ARG		410	-27.926				35.73	6
157	25	ATOM	1147		ARG		410	-29.234				33.17	7
111		ATOM	1148	NH2	ARG		410	-27.095				32.70	7
I.U		ATOM	1149	С	ARG			-25.688				46.67	6
Just		ATOM	1150	0	ARG			-25.859				41.78	8
1		ATOM	1151	N	LYS			-24.602				52.99	7
lah i. z	30	MOTA	1152	CA	LYS			-23.471				58.32	6
14		ATOM	1153	CB	LYS		411	-23.684				64.99	6
		ATOM	1154	CG	LYS			-24.998				70.48	6
		ATOM	1155	CD	LYS		411	-25.070				77.18	6
W		ATOM	1156	CE	LYS		411	-26.272				84.30	6
IJ	35	ATOM	1157	NZ	LYS		411	-26.286				86.48	7
100		ATOM	1158	С	LYS		411	-23.172				56.66	6
ığ.		ATOM	1159	0	LYS	В	411	-23.574	4 60.19			55.47	8
1148		ATOM	1160	N	HIS		412	-22.458				54.67	7
		ATOM	1161	CA	HIS	В	412	-22.019				48.67	6
	40	ATOM	1162	CB	HIS		412	-21.500				43.14	6
		ATOM	1163	CG	HIS	В	412	-22.559	9 63.50			41.36	6
		ATOM	1164	CD2	HIS	В	412	-23.159				35.44	6
		ATOM	1165	ND1	HIS	В	412	-23.163				38.19	7
		ATOM	1166	CE1	HIS	В	412	-24.07				34.75	6
	45	ATOM	1167	NE2	HIS			-24.090				35.52	7
		ATOM	1168	С	HIS	В	412	-20.89	4 60.59			46.35	6
		ATOM	1169	0	HIS	В	412	-20.218	3 60.8	92 30.644		42.73	8
		ATOM	1170	N	HIS	В	413	-20.708				48.92	7
		ATOM	1171	CA	HIS	В	413	-19.593	3 58.6	L4 29.371		53.15	6
	50	ATOM	1172	CB	HIS	В	413	-20.022	2 57.1	47 29.421		55.27	6
		ATOM	1173	CG	HIS	В	413	-20.81	4 56.82	23 30.636	1.00	58.77	6
		ATOM	1174	CD2	HIS	В	413	-22.019	9 56.22	23 30.822	1.00	61.65	6
		ATOM	1175	ND1	HIS	В	413	-20.360	57.1	59 31.921	1.00	60.31	7
		ATOM	1176	CE1	HIS	В	413	-21.26	7 56.7	32.809	1.00	63.01	6
	55	ATOM	1177		HIS			-22.27	0 56.1	93 32.171	1.00	62.93	7
		ATOM	1178	С	HIS	В	413	-18.42	6 58.8	52 28.438	1.00	53.19	6
		ATOM	1179	0	HIS	В	413	-17.97	5 57.9	96 27.699	1.00	54.93	8
		ATOM	1180	N	VAL	В	414	-17.97	0 60.1	13 28.521	1.00	53.77	7

	5	ATOM	1181	CA	VAL	В	414	-16.845	60.674	27.788	1.00	51.06	6
		ATOM	1182	CB	VAL		414	-17.317	61.498	26.586		51.49	6
								-16.133	62.122	25.891		45.22	6
		ATOM	1183		VAL		414					52.67	6
		MOTA	1184		VAL		414	-18.095	60.631	25.617			
		MOTA	1185	С	VAL		414	-16.096	61.557	28.775		54.28	6
	10	ATOM	1186	0	VAL			-16.700	62.283	29.574		55.49	8
		MOTA	1187	N	THR	В	415	-14.770	61.466	28.742		56.28	7
		MOTA	1188	CA	THR	В	415	-13.919	62.234	29.669	1.00	57.83	6
		ATOM	1189	CB	THR	В	415	-12.488	61.686	29.658	1.00	59.64	6
		ATOM	1190	OG1	THR	В	415	-11.618	62.572	30.373	1.00	66.69	8
	15	ATOM	1191	CG2	THR	В	415	-11.988	61.483	28.227	1.00	59.42	6
		ATOM	1192	С	THR	В	415	-13.840	63.726	29.352	1.00	56.98	6
		ATOM	1193	0	THR		415	-13.987	64.135	28.216	1.00	55.70	8
		ATOM	1194	N	HIS		416	-13.598	64.522	30.387	1.00	57.44	7
		ATOM	1195	CA	HIS		416	-13.485	65.972	30.237		57.34	6
	20	ATOM	1196	CB	HIS		416	-12.114	66.326	29.653		61.35	6
	20	ATOM	1197	CG	HIS			-10.968	65.931	30.513		69.78	6
								-9.930	65.082	30.307		71.42	6
		ATOM	1198		HIS		416					72.49	7
		MOTA	1199		HIS		416	-10.756	66.480	31.787			6
las J		MOTA	1200		HIS			-9.631	65.973	32.281		75.50	7
D	25	MOTA	1201		HIS			-9.120	65.131	31.408		73.91	
111		MOTA	1202	С	HIS		416	-14.560	66.515	29.320		53.79	6
(D)		ATOM	1203	0	HIS			-14.334	67.477	28.591		52.81	8
lust.		ATOM	1204	N	PHE		417	-15.746	65.921	29.372		48.05	7
V		ATOM	1205	CA	PHE		417	-16.841	66.329	28.505		47.99	6
ledi-	30	ATOM	1206	CB	PHE	В	417	-18.152	65.694	28.937		46.11	6
14		ATOM	1207	CG		В	417	-19.233	65.781	27.898		44.27	6
11		ATOM	1208	CD1	PHE	В	417	-19.280	64.856	26.870		41.79	6
100		ATOM	1209	CD2	PHE	В	417	-20.118	66.846	27.893		40.23	6
الدا		ATOM	1210	CE1	PHE	В	417	-20.233	64.959	25.869	1.00	44.30	6
1,0	35	ATOM	1211	CE2	PHE	В	417	-21.072	66.955	26.893	1.00	36.80	6
127		ATOM	1212	CZ	PHE	В	417	-21.119	66.016	25.866	1.00	40.69	6
:0		ATOM	1213	С	PHE	В	417	-17.020	67.833	28.423	1.00	46.69	6
+D		ATOM	1214	0	PHE	В	417	-16.799	68.423	27.380	1.00	43.35	8
		ATOM	1215	N	TRP	В	418	-17.448	68.452	29.516	1.00	45.14	7
	40	ATOM	1216	CA	TRP			-17.681	69.889	29.508	1.00	44.89	6
		ATOM	1217	CB			418	-18.045	70.398	30.898	1.00	42.24	6
		ATOM	1218	CG	TRP		418	-18.162	71.905	31.018	1.00	47.11	6
		ATOM	1219		TRP			-19.298	72.699	30.620		46.98	6
			1220	CE2			418	-18.953	74.061	30.850		48.94	6
	45	ATOM		CE3				-20.560	72.401	30.086		45.23	6
	43	ATOM	1221					-17.223	72.778	31.462		46.24	6
		ATOM	1222	CD1					74.071	31.368		50.63	7
		ATOM	1223	NE1				-17.690					6
		ATOM	1224	CZ2				-19.819	75.109	30.571		45.46	
		ATOM	1225	CZ3			418	-21.422	73.447	29.809		44.50	6
	50	ATOM	1226	CH2			418	-21.065	74.777	30.039		47.55	6
		MOTA	1227	С			418	-16.502	70.662	28.956		43.88	6
		ATOM	1228	0			418	-16.671	71.424	27.986		43.17	8
		ATOM	1229	N			419	-15.292	70.490	29.519		43.55	7
		ATOM	1230	CD	PRO	В	419	-14.967	69.551	30.599		41.52	6
	55	ATOM	1231	CA	PRO	В	419	-14.120	71.223	29.011		41.48	6
		ATOM	1232	CB	PRO	В	419	-12.956	70.582	29.724		39.21	6
		ATOM	1233	CG	PRO	В	419	-13.521	69.703	30.774		39.25	6
		ATOM	1234	С	PRO	В	419	-14.035	71.067	27.479	1.00	36.28	6

	5	ATOM	1235	0	PRO	В	419	-13.690	72.001	26.754	1.00	37.08	8
	,	ATOM	1236	N	LYS		420	-14.330	69.871	26.976		35.96	7
		ATOM	1237	CA	LYS		420	-14.278	69.609	25.538		40.82	6
		ATOM	1238	CB	LYS		420	-14.452	68.103	25.271		40.78	6
			1239	CG	LYS		420	-13.349	67.214	25.830		48.62	6
1	Λ	ATOM	1239	CD	LYS		420	-13.565	65.746	25.480		55.12	6
1	.0	ATOM						-12.427	64.892	26.017		53.26	6
		ATOM	1241	CE	LYS		420			25.608		52.69	7
		ATOM	1242	NZ	LYS		420	-12.582	63.457	24.875		40.29	6
		ATOM	1243	С	LYS		420	-15.414	70.374			39.66	8
	_	ATOM	1244	0	LYS			-15.225	71.015	23.851			7
1	5	ATOM	1245	N	LEU		421	-16.591	70.300	25.499		38.33	
		MOTA	1246	CA	LEU		421	-17.796	70.958	25.001		37.60	6
		ATOM	1247	CB	LEU		421	-18.970	70.702	25.965		43.66	6
		ATOM	1248	CG	LEU		421	-20.370	70.850	25.418		46.50	6
		ATOM	1249		LEU			-20.529	69.890	24.255		45.15	6
2	20	ATOM	1250	CD2	LEU	В	421	-21.383	70.538	26.486		51.31	6
		ATOM	1251	С	LEU		421	-17.547	72.452	24.823		39.59	6
		ATOM	1252	0	LEU	В	421	-17.975	73.035	23.836		40.66	8
		ATOM	1253	N	LEU	В	422	-16.847	73.059	25.780		39.57	7
1.2		ATOM	1254	CA	LEU	В	422	-16.534	74.478	25.715		38.63	6
(D)	25	ATOM	1255	CB	LEU	В	422	-15.829	74.936	26.992		41.79	6
TU		ATOM	1256	CG	LEU	В	422	-16.714	75.149	28.191	1.00	42.74	6
£Q.		ATOM	1257	CD1	LEU	В	422	-15.911	75.685	29.360	1.00	42.89	6
- Peril		ATOM	1258	CD2	LEU	В	422	-17.783	76.162	27.813	1.00	39.27	6
14		ATOM	1259	С	LEU	В	422	-15.677	74.788	24.513	1.00	40.47	6
1.4	30	ATOM	1260	0	LEU	В	422	-15.823	75.846	23.917	1.00	47.83	8
114		ATOM	1261	N	MET		423	-14.789	73.853	24.168	1.00	34.27	7
1)		ATOM	1262	CA	MET		423	-13.907	74.019	23.024	1.00	35.25	6
1		ATOM	1263	CB			423	-12.920	72.858	22.922	1.00	32.56	6
1,1		ATOM	1264	CG	MET		423	-12.013	72.703	24.125	1.00	40.70	6
	35	ATOM	1265	SD	MET	В	423	-10.345	72.007	23.784	1.00	47.65	16
7,50		ATOM	1266	CE			423	-10.770	70.538	22.761	1.00	47.16	6
10		ATOM	1267	C			423	-14.709	74.100	21.738	1.00	35.13	6
111		ATOM	1268	ō	MET		423	-14.341	74.807	20.803	1.00	29.85	8
		ATOM	1269	N	LYS			-15.811	73.361	21.704	1.00	31.56	7
	40	ATOM	1270	CA	LYS		424	-16.676	73.354	20.544	1.00	32.29	6
	10	ATOM	1271	CB	LYS		424	-17.783	72.316	20.736		30.56	6
		ATOM	1272	CG	LYS		424	-17.257	70.879	20.843		30.07	6
		ATOM	1273	CD	LYS			-16.444	70.510	19.611	1.00	33.22	6
		ATOM	1274	CE	LYS		424	-15.795	69.136	19.706		28.75	6
	45	ATOM	1275	NZ	LYS		424	-14.655	69.067	20.678		31.01	7
	+3	ATOM	1276	C	LYS			-17.248	74.754	20.304		29.26	6
			1277	0	LYS			-17.439	75.149	19.166		30.22	8
		ATOM		N			425	-17.495	75.499	21.385		23.53	7
		ATOM	1278		VAL		425	-18.014	76.852	21.278		28.91	6
	50	ATOM	1279	CA		В	425	-18.278	77.458	22.663		29.44	6
	50	MOTA	1280	CB	VAL			-18.633	78.915	22.547		28.81	6
		ATOM	1281		VAL				76.733	23.354		31.22	6
		ATOM	1282		VAL			-19.401				32.03	6
		ATOM	1283	С			425	-17.001	77.682	20.498			8
		ATOM	1284	0	VAL		425	-17.368	78.465	19.629		31.95	7
	55	ATOM	1285	N	THR		426	-15.721	77.508	20.827		33.61	6
		ATOM	1286	CA	THR		426	-14.645	78.221	20.137		30.76	
		ATOM	1287	CB	THR		426	-13.270	77.912	20.761		32.34	6
		ATOM	1288	OG1	THR	В	426	-13.073	78.697	21.941	1.00	33.07	8

	5	ATOM	1289	CG2	THR	В	426	-12.153	78.174	19.782		25.40	6
		ATOM	1290	C	THR	В	426	-14.677	77.742	18.706		32.53	6
		ATOM	1291	0	THR	В	426	-14.639	78.530	17.763		35.19	8
		ATOM	1292	N	ASP	В	427	-14.749	76.425	18.566		28.83	7
		ATOM	1293	CA	ASP	В	427	-14.796	75.807	17.257	1.00	35.12	6
	10	ATOM	1294	CB	ASP	В	427	-15.096	74.302	17.380	1.00	39.14	6
		ATOM	1295	CG	ASP	В	427	-13.910	73.496	17.806	1.00	45.80	6
		ATOM	1296	OD1	ASP	В	427	-12.786	73.774	17.348	1.00	41.97	8
		ATOM	1297		ASP		427	-14.064	72.517	18.583	1.00	50.06	8
		ATOM	1298	С	ASP		427	-15.883	76.502	16.429	1.00	33.94	6
	15	ATOM	1299	0	ASP	В	427	-15.673	76.815	15.262	1.00	38.02	8
		ATOM	1300	N	LEU		428	-17.040	76.741	17.048	1.00	27.15	7
		ATOM	1301	CA	LEU		428	-18.154	77.388	16.367	1.00	29.99	6
		ATOM	1302	CB	LEU		428	-19.448	77.190	17.168	1.00	22.49	6
		ATOM	1303	CG	LEU		428	-20.086	75.818	17.089	1.00	25.54	6
	20	ATOM	1304		LEU		428	-21.282	75.729	18.012	1.00	20.60	6
	20	ATOM	1305	CD2	LEU		428	-20.509	75.564	15.651	1.00	17.24	6
		ATOM	1306	C	LEU		428	-17.901	78.863	16.103	1.00	28.94	6
		ATOM	1307	0	LEU		428	-18.328	79.388	15.076	1.00	31.26	8
100		ATOM	1308	N	ARG		429	-17.213	79.524	17.035	1.00	27.64	7
100	25	ATOM	1309	CA	ARG		429	-16.894	80.937	16.883		28.13	6
fu	23	ATOM	1310	CB	ARG			-16.274	81.507	18.160		29.59	6
10		ATOM	1311	CG	ARG			-17.246	81.752	19.302		34.85	6
Seal.		ATOM	1312	CD	ARG			-16.626	82.653	20.372		47.18	6
11/4		ATOM	1313	NE	ARG		429	-17.373	82.714	21.620		57.93	7
į.i.	30	ATOM	1314	CZ	ARG		429	-18.632	83.124	21.716		63.62	6
100	30	ATOM	1314		ARG		429	-19.263	83.579	20.622		60.71	7
61		ATOM	1316		ARG		429	-19.238	83.130	22.916		62.38	7
1150		ATOM	1317	C	ARG			-15.930	81.146	15.728		29.81	6
1al		ATOM	1318	0	ARG			-16.101	82.061	14.933		30.81	8
	35	ATOM	1319	N	MET		430	-14.908	80.295	15.670		29.64	7
112	33	ATOM	1320	CA	MET			-13.920	80.343	14.614		34.72	6
100		ATOM	1321	CB	MET		430	-12.939	79.192	14.763		34.97	6
110		ATOM	1322	CG	MET		430	-11.787	79.431	15.689		45.34	6
		ATOM	1323	SD	MET		430	-10.729	80.768	15.158		52.55	16
	40	ATOM	1324	CE			430	-10.070	80.157	13.610		55.56	6
	70	ATOM	1325	C	MET		430	-14.638	80.217	13.284		34.01	6
		ATOM	1326	0	MET			-14.395	80.996	12.385		37.29	8
		ATOM	1327	N			431	-15.516	79.217	13.176		29.99	7
		ATOM	1328	CA			431	-16.296	78.992	11.963		28.82	6
	45	ATOM	1329	CB			431	-17.391	77.929	12.177		27.39	6
	43		1330		ILE			-18.314	77.841	10.959		23.87	6
		ATOM	1331	CG1				-16.784	76.555	12.449		25.56	6
		ATOM			ILE			-17.826	75.464	12.498		17.29	6
		ATOM	1332				431	-16.953	80.288	11.538		29.49	6
	50	ATOM	1333	С	ILE		431	-16.837	80.725	10.398		24.19	8
	50	ATOM	1334	O N	GLY		431	-17.657	80.904	12.474		25.25	7
		ATOM	1335					-18.357	82.142	12.179		30.38	6
		ATOM	1336	CA			432			11.725		32.75	6
		ATOM	1337	С			432	-17.395	83.209 83.740	10.637		36.38	8
		ATOM	1338	0			432	-17.531		12.586		26.77	7
	55	ATOM	1339	N			433	-16.431	83.522	12.299		26.48	6
		ATOM	1340	CA	ALA		433	-15.407	84.514 84.338	13.253		19.90	6
		ATOM	1341	CB			433	-14.240		10.867		30.73	6
		ATOM	1342	С	ALA	B	433	-14.905	84.433	10.007	1.00	50.75	_

	5	ATOM	1343	0	ALA	В	433	-14.849	85.432	10.171	1.00	31.60	8
		ATOM	1344	N	CYS	В	434	-14.534	83.246	10.439	1.00	33.22	7
		ATOM	1345	CA	CYS	В	434	-14.023	83.021	9.120	1.00	34.34	6
		ATOM	1346	CB	CYS	В	434	-13.553	81.661	9.226	1.00	35.20	6
		ATOM	1347	SG	CYS	В	434	-12.412	81.249	8.444	1.00	54.48	16
	10	ATOM	1348	С	CYS	В	434	-15.106	83.116	8.062	1.00	34.09	6
		ATOM	1349	Ō	CYS			-14.844	83.555	6.952	1.00	34.89	8
		ATOM	1350	N	HIS			-16.318	82.699	8.394	1.00	34.30	7
		ATOM	1351	CA	HIS			-17.395	82.762	7.443	1.00	35.44	6
		ATOM	1352	CB	HIS			-18.700	82.404	8.103	1.00	31.76	6
	15	ATOM	1353	CG	HIS			-19.845	82.425	7.149	1.00	32.03	6
	10	ATOM	1354		HIS			-20.483	81.419	6.515	1.00	28.61	6
		ATOM	1355		HIS			-20.345	83.600	6.607	1.00	28.48	7
		ATOM	1356		HIS			-21.241	83.293	5.672		33.27	6
		ATOM	1357		HIS			-21.341	81.977	5.605		31.57	7
	20	ATOM	1358	C	HIS			-17.528	84.152	6.878		32.74	6
	20	ATOM	1359	Ö	HIS			-17.842	84.326	5.715		32.87	8
		ATOM	1360	N	ALA			-17.315	85.121	7.758		31.01	7
		ATOM	1361	CA	ALA			-17.376	86.520	7.405		29.91	6
3 750)		ATOM	1362	CB	ALA			-17.008	87.352	8.618		21.23	6
0	25	ATOM	1363	C	ALA			-16.393	86.782	6.266		33.86	6
111	23	ATOM	1364	Ö	ALA			-16.734	87.398	5.257		36.10	8
10		ATOM	1365	N			437	-15.162	86.307	6.448		35.19	7
inh.		ATOM	1366	CA			437	-14.122	86.484	5.445		33.03	6
34		ATOM	1367	CB			437	-12.882	85.688	5.847		35.31	6
finds	30	ATOM	1368	OG			437	-11.855	85.824	4.879		44.99	8
34.5	30	ATOM	1369	C			437	-14.642	85.993	4.108		38.39	6
ž)		ATOM	1370	Ö			437	-14.700	86.730	3.127		37.54	8
1000		ATOM	1371	N			438	-15.008	84.719	4.096		37.32	7
LU		ATOM	1372	CA	ARG			-15.526	84.068	2.908		39.30	6
113	35	ATOM	1373	CB	ARG		438	-16.019	82.660	3.259		42.97	6
133	33	ATOM	1374	CG	ARG			-14.910	81.673	3.590		41.72	6
10		ATOM	1375	CD			438	-14.044	81.488	2.356		45.23	6
ŧΩ		ATOM	1376	NE			438	-14.781	80.936	1.235		45.66	7
		ATOM	1377	CZ	ARG			-14.482	81.175	-0.040		49.71	6
	40	ATOM	1378		ARG			-13.458	81.977	-0.347		50.91	7
	40	ATOM	1379		ARG			-15.219	80.619	-1.002		46.86	7
		ATOM	1380	C			438	-16.659	84.859	2.287		42.37	6
		ATOM	1381	0			438	-16.841	84.832	1.072		40.58	8
		ATOM	1382	N			439	-17.417	85.575	3.117		42.25	7
	45	ATOM	1383	CA			439	-18.531	86.354	2.614		42.81	6
	43	ATOM	1384	CB			439	-19.198	87.132	3.731		42.18	6
		ATOM	1385	CG	PHE			-20.487	87.769	3.323		42.48	6
		ATOM	1386		PHE			-21.535	86.981	2.912		47.09	6
		ATOM	1387		PHE			-20.638	89.141	3.334		39.76	6
	50		1388		PHE			-22.735	87.543	2.527		49.17	6
	30	ATOM ATOM	1389		PHE			-21.851	89.717	2.944		45.10	6
				CZ			439	-22.901	88.911	2.538		46.36	6
		ATOM	1390				439	-18.016	87.319	1.581		44.79	6
		ATOM	1391 1392	C 0			439	-18.514	87.354	0.465		40.26	8
	55	ATOM	1392	N	LEU			-17.021	88.117	1.987		42.77	7
	33	ATOM	1394	CA			440	-16.415	89.115	1.109		42.96	6
		ATOM			LEU			-15.169	89.718	1.768		37.19	6
		ATOM	1395	CB CG			440	-15.109	90.588	2.967		36.97	6
		ATOM	1396	CG	DE O	D	440	10.11	20.200	2.501	1.00		-

	5	ATOM	1397	CD1	LEU	В	440	-14.219	91.352	3.402	1.00	33.65	6
		ATOM	1398	CD2	LEU	В	440	-16.577	91.591	2.574	1.00	35.42	6
		ATOM	1399	С	LEU	В	440	-16.099	88.561	-0.273	1.00	45.47	6
		ATOM	1400	ō	LEU			-16.631	89.059	-1.265	1.00	52.48	8
		ATOM	1401	N	HIS			-15.238	87.549	-0.345	1.00	49.15	7
	10	ATOM	1402	CA	HIS		441	-14.929	86.956	-1.632	1.00	54.76	6
	10	ATOM	1403	CB	HIS			-14.150	85.700	-1.448	1.00		6
			1404	CG	HIS		441	-12.713	85.934	-1.230	1.00		6
		ATOM	1404		HIS		441	-11.602	85.418	-1.812	1.00		6
		ATOM					441	-12.245	86.850	-0.273	1.00		7
	1.0	ATOM	1406		HIS			-10.916	86.847	-0.309	1.00		6
	15	ATOM	1407		HIS				85.993	-1.228	1.00		7
		ATOM	1408		HIS		441	-10.512	86.633	-2.301	1.00		6
		ATOM	1409	C	HIS			-16.217		-3.465	1.00		8
		ATOM	1410	0	HIS		441	-16.418	86.938	-1.553	1.00		7
		ATOM	1411	N	MET			-17.106	85.997		1.00		6
	20	ATOM	1412	CA	MET		442	-18.399	85.652	-2.106		55.93	
		MOTA	1413	CB	MET			-19.340	85.162	-1.008			6 6
		ATOM	1414	CG	MET		442	-18.991	83.796	-0.456	1.00		
		ATOM	1415	SD	MET		442	-20.310	82.994	0.505		60.99	16
15		ATOM	1416	CE	MET			-20.525	84.203	1.827	1.00		6
10	25	ATOM	1417	С	MET			-18.991	86.879	-2.785		60.31	6
17.5		MOTA	1418	0	MET		442	-19.646	86.778	-3.817		58.18	8
10		MOTA	1419	N	LYS			-18.731	88.045	-2.213		61.45	7
frah.		ATOM	1420	CA	LYS		443	-19.267	89.268	-2.758		64.90	6
N		ATOM	1421	CB	LYS		443	-19.182	90.358	-1.704		64.40	6
find.	30	ATOM	1422	CG	LYS		443	-20.160	91.449	-1.982		69.12	6
4		ATOM	1423	CD			443	-19.763	92.673	-1.306		71.14	6
11		ATOM	1424	CE	LYS			-20.508	92.993	-0.491		73.43	6
42		ATOM	1425	NZ	LYS			-20.174	94.242	0.151		67.97	7
1.1		ATOM	1426	С	LYS			-18.528	89.704	-4.020		67.29	6
W	35	ATOM	1427	0	LYS	В	443	-18.979	90.586	-4.731		67.90	8
0		ATOM	1428	N	VAL	В	444	-17.383	89.075	-4.285		66.57	7
10		ATOM	1429	CA	VAL	В	444	-16.589	89.418	-5.455		64.76	6
1,62		ATOM	1430	CB	VAL	В	444	-15.097	89.568	-5.082		62.76	6
		ATOM	1431	CG1	VAL	В	444	-14.269	89.857	-6.298		64.00	6
	40	ATOM	1432	CG2	VAL	В	444	-14.905	90.678	-4.042		59.27	6
		ATOM	1433	С	VAL	В	444	-16.800	88.397	-6.569		68.61	6
		ATOM	1434	0	VAL	В	444	-16.968	88.774	-7.729		70.60	8
		ATOM	1435	N	GLU	В	445	-16.812	87.118	-6.219		70.71	7
		ATOM	1436	CA	GLU	В	445	-16.951	86.033	-7.197		71.45	6
	45	ATOM	1437	CB	GLU	В	445	-16.169	84.809	-6.712		72.36	6
		ATOM	1438	CG	GLU	В	445	-14.736	85.090	-6.392		40.00	6
		ATOM	1439	CD	GLU	В	445	-13.998	83.890	-5.851		40.00	6
		ATOM	1440	OE1	GLU	В	445	-14.587	82.798	-5.665		40.00	8
		ATOM	1441	OE2	GLU	В	445	-12.775	83.995	-5.580		40.00	8
	50	ATOM	1442	С	GLU	В	445	-18.375	85.574	-7.422		71.46	6
		ATOM	1443	0	GLU	В	445	-18.605	84.542	-8.064		73.02	8
		ATOM	1444	N	CYS	В	446	-19.328	86.333	-6.900	1.00	71.12	7
		ATOM	1445	CA	CYS		446	-20.694	85.942	-7.062		70.83	6
		ATOM	1446	CB	CYS		446	-21.196	85.230	-5.784		71.05	6
	55	ATOM	1447	SG	CYS		446	-20.296	83.720	-5.349	1.00	72.83	16
		ATOM	1448	С	CYS		446	-21.563	87.135	-7.386	1.00	71.91	6
		ATOM	1449	ō	CYS			-21.307	88.244	-6.911	1.00	72.06	8
		ATOM	1450	N			447	-22.550	86.928	-8.256	1.00	73.12	7
		-											

	5	ATOM	1505	0	PRO	В	453	-29.7	00	90.206	3.345	1.00	54.17	8
		ATOM	1506	N	LEU	В	454	-31.8	07	89.458	3.631	1.00	51.21	7
		ATOM	1507	CA	LEU		454	-31.5	38	88.945	4.948	1.00	47.17	6
		ATOM	1508	CB			454	-32.5	550	87.858	5.330	1.00	44.44	6
		ATOM	1509	CG	LEU		454	-32.3	347	87.412	6.748	1.00	41.33	6
	10	ATOM	1510		LEU		454	-31.9		88.589	7.631	1.00	35.93	6
	10	ATOM	1511		LEU		454	-33.5		86.732	7.239	1.00	34.79	6
				C	LEU		454	-30.0		88.443	4.928		42.25	6
		ATOM	1512					-29.3		88.774	5.812		40.82	8
		MOTA	1513	0	LEU						3.885		39.29	7
		ATOM	1514	N			455	-29.7		87.707			41.81	6
	15	ATOM	1515	CA			455	-28.3		87.204	3.770		47.22	6
		ATOM	1516	CB	PHE			-28.3		86.536	2.418			
		ATOM	1517	CG	PHE			-26.8		85.836	2.292		56.97	6
		ATOM	1518		PHE			-26.		84.915	3.247		57.23	6
		ATOM	1519	CD2	PHE	В	455	-25.		86.094	1.236		59.40	6
	20	ATOM	1520	CE1	PHE	В	455	-25.2	225	84.234	3.153		56.58	6
		ATOM	1521	CE2	PHE	В	455	-24.	720	85.409	1.134		61.80	6
		ATOM	1522	CZ	PHE	В	455	-24.	360	84.481	2.103		59.94	6
		ATOM	1523	С	PHE	В	455	-27.	100	88.386	3.923	1.00	45.12	6
		ATOM	1524	0	PHE	В	455	-26.	657	88.450	4.889	1.00	39.95	8
10	25	ATOM	1525	N	LEU	В	456	-27.	439	89.303	2.949	1.00	43.92	7
173		ATOM	1526	CA	LEU	В	456	-26.	597	90.503	2.947	1.00	44.08	6
100		ATOM	1527	CB	LEU			-27.	001	91.440	1.802	1.00	50.20	6
Int.		ATOM	1528	CG	LEU		456	-26.		91.155	0.432	1.00	55.79	6
1.1		ATOM	1529		LEU		456	-27.		92.082	-0.591	1.00	54.70	6
1.4.	30		1530		LEU			-24.		91.345	0.494		53.01	6
1	30	ATOM ATOM	1531	CDZ	LEU		456	-26.		91.245	4.264		44.65	6
ii.				0	LEU			-25.		91.540	4.886		45.93	8
12		ATOM	1532		GLU			-27.		91.268	4.265		44.56	7
Li		ATOM	1533	N				-28.		92.016	5.497		46.37	6
W	2.5	ATOM	1534	CA	GLU			-27.		91.452	6.628		43.60	6
£	35	ATOM	1535	С	GLU		457	-27.		92.223	7.339		42.69	8
100		ATOM	1536	0	GLU					91.879	5.855		50.16	6
-0		ATOM	1537	CB	GLU		457	-29.			6.954		20.00	6
-		MOTA	1538	CG	GLU		457	-30.		92.849			20.00	6
		ATOM	1539	CD	GLU		457	-31.		93.338	6.782			8
	40	ATOM	1540	OE1				-32.		92.932	5.779		20.00	8
		ATOM	1541	OE2	GLU		457	-32.		94.156	7.638		20.00	7
		ATOM	1542	N	VAL	В	458	-27.		90.413	7.281		43.21	
		ATOM	1543	CA	VAL		458	-26.		89.739	8.351		44.98	6
		ATOM	1544	CB	VAL	В	458	-27.		88.255	8.432		44.83	6
	45	ATOM	1545	CG1	VAL	В	458	-26.		87.623	9.646		49.72	6
		ATOM	1546	CG2	VAL	В	458	-28.	562	88.086	8.474		40.89	6
		ATOM	1547	С	VAL	В	458	-25.	190	89.822	8.311		42.72	6
		ATOM	1548	0	VAL	В	458	-24.	551	90.179	9.303	1.00	42.88	8
		ATOM	1549	N	PHE	В	459	-24.	605	89.488	7.180	1.00	44.53	7
	50	ATOM	1550	CA	PHE	В	459	-23.	165	89.480	7.077	1.00	48.18	6
	-	ATOM	1551	СВ	PHE			-22.	747	88.457	6.065	1.00	43.60	6
		ATOM	1552	CG	PHE	В		-23.	167	87.116	6.441	1.00	40.79	6
		ATOM	1553		PHE			-24.		86.750	6.368	1.00	41.01	6
		ATOM	1554	CD2	PHE			-22.		86.286	7.009	1.00	39.48	6
	55	ATOM	1555	CE1				-24.		85.540	6.889		40.62	6
	دد	ATOM	1556	CE2				-22.		85.091	7.527		36.87	6
		ATOM	1557	CEZ	PHE			-23.		84.711	7.455		36.39	6
		ATOM	1558	C			459	-22.		90.758	6.623		52.71	6
		HION	1000	_	£ 11E	۵	400			- 0 0				

	5	ATOM	4035	C11	Т3	K	1	-26.708	75.670	7.834		23.12	6
		ATOM	4036	C12	Т3	K	1	-24.521	78.610	5.376		19.67	6
		ATOM	4037	C13	Т3	K	1	-29.211	75.830	8.626		18.97	6
		ATOM	4038	C15	Т3	K	1	-29.181	74.567	9.488		19.32	6
		ATOM	4039	C17	Т3	K	1	-30.440	74.343	10.264	1.00	19.02	6
	10	ATOM	4040	11	Т3	K	1	-27.868	77.342	3.316	1.00	25.29	53
		ATOM	4041	12	Т3	K	1	-22.732	79.619	0.850	1.00	26.49	53
		ATOM	4042	13	т3	K	1	-23.602	75.792	7.334	1.00	25.67	53
		ATOM	4043	N1	Т3	K	1	-28.680	73.342	8.762	1.00	15.12	7
		ATOM	4044	01	Т3	K	1	-22.742	81.265	3.443	1.00	21.79	8
	15	ATOM	4045	02	Т3	K	1	-25.267	76.388	4.595	1.00	22.05	8
		ATOM	4046	03	Т3	K	1	-30.816	73.159	10.382	1.00	20.38	8
		ATOM	4047	04	Т3	K	1	-31.028	75.359	10.729	1.00	20.16	8
		TER											
		ATOM	1	С	LYS	х	686	13.868	40.176	48.888	1.00	40.00	6
	20	ATOM	2	ō	LYS			13.914	40.120	47.639	1.00	40.00	8
	20	ATOM	3	N	LYS			14.374	42.245	50.489	1.00	40.00	7
		ATOM	4	CA	LYS			14.937	41.070	49.710	1.00	40.00	6
		ATOM	5	N	HIS			13.038	39.527	49.705	1.00	40.00	7
/25		ATOM	6	CA	HIS			11.891	38.518	49.521	1.00	40.00	6
	25	ATOM	7	CB	HIS			10.639	39.000	50.212	1.00	40.00	6
111		ATOM	8	CG	HIS			10.981	39.526	51.563	1.00	40.00	6
111		ATOM	9		HIS		687	11.021	38.908	52.753	1.00	40.00	6
3,00		ATOM	10		HIS		687	11.354	40.844	51.754	1.00	40.00	7
10		ATOM	11		HIS			11.614	40.994	53.034	1.00	40.00	6
800	30	ATOM	12		HIS			11.422	39.847	53.646	1.00	40.00	7
314	50	ATOM	13	С	HIS		687	11.183	38.108	48.208	1.00	40.00	6
11		ATOM	14	ō			687	11.674	38.361	47.094	1.00	40.00	8
100		ATOM	15	N	LYS			10.064	37.458	48.649	1.00	40.00	7
M		ATOM	16	CA	LYS		688	8.911	36.858	47.931	1.00	40.00	6
144	35	ATOM	17	CB	LYS	Х	688	8.292	37.850	46.968	1.00	40.00	6
		ATOM	18	C	LYS			9.246	35.573	47.161	1.00	40.00	6
10		ATOM	19	0	LYS		688	9.319	34.473	47.722	1.00	40.00	8
10		ATOM	20	N			689	9.426	35.754	45.865	1.00	40.00	7
		ATOM	21	CA			689	9.661	34.640	44.924	1.00	40.00	6
	40	ATOM	22	CB	ILE	Х	689	9.731	35.167	43.498	1.00	40.00	6
		ATOM	23		ILE			9.638	34.053	42.453	1.00	40.00	6
		ATOM	24	CG1	ILE	Х	689	8.597	36.141	43.176	1.00	40.00	6
		ATOM	25	CD1	ILE	Х	689	8.250	36.183	41.688	1.00	40.00	6
		ATOM	26	С	ILE	Х	689	10.954	33.869	45.228	1.00	40.00	6
	45	ATOM	27	0	ILE	Х	689	10.920	32.657	45.511	1.00	40.00	8
		ATOM	28	N			690	12.065	34.579	45.140	1.00	40.00	7
		ATOM	29	CA	LEU	Х	690	13.391	33.996	45.397	1.00	40.00	6
		ATOM	30	CB	LEU	Х	690	14.349	35.043	45.892	1.00	40.00	6
		ATOM	31	CG	LEU	Х	690	14.450	36.168	44.906	1.00	40.00	6
	50	ATOM	32	CD1	LEU	Х	690	15.397	37.261	45.363	1.00	40.00	6
		ATOM	33	CD2	LEU	X	690	14.940	35.695	43.540	1.00	40.00	6
		ATOM	34	C			690	13.271	32.999	46.466	1.00	40.00	6
		ATOM	35	0	LEU	Х	690	13.633	31.832	46.315	1.00	40.00	8
		ATOM	36	N			691	12.773	33.472	47.541	1.00	40.00	7
	55	ATOM	37	CA			691	12.557	32.559	48.569		40.00	6
		ATOM	38	CB	HIS	X	691	11.729	33.212	49.658	1.00	40.00	6
		ATOM	39	CG	HIS	X	691	12.588	34.116	50.564		40.00	6
		ATOM	40		HIS			13.648	33.852	51.385	1.00	40.00	6

	5	ATOM	41	ND1	HIS	Χ	691	12.359	35.484	50.669		40.00	7
		ATOM	42	CE1	HIS	Χ	691	13.242	35.991	51.513		40.00	6
		ATOM	43	NE2	HIS	Х	691	14.016	35.031	51.949		40.00	7
		ATOM	44	С	HIS	X	691	11.954	31.331	47.861		40.00	6
		ATOM	45	0	HIS	Χ	691	12.505	30.240	47.882		40.00	8
1	10	ATOM	46	N	ARG	Х	692	10.839	31.494	47.167		40.00	7
		ATOM	47	CA	ARG	Х	692	10.169	30.333	46.518	1.00	40.00	6
		ATOM	48	CB	ARG	Х	692	9.118	30.800	45.517		40.00	6
		ATOM	49	С	ARG	Х	692	11.153	29.402	45.752	1.00	40.00	6
		ATOM	50	0	ARG	Х	692	11.030	28.168	45.779	1.00	40.00	8
	15	ATOM	51	N	LEU	Х	693	12.117	30.000	45.072	1.00	40.00	7
		ATOM	52	CA	LEU	Х	693	13.078	29.252	44.226	1.00	40.00	6
		ATOM	53	CB	LEU	Х	693	13.784	30.210	43.274	1.00	40.00	6
		ATOM	54	CG	LEU	Х	693	12.796	31.012	42.432	1.00	40.00	6
		ATOM	55	CD1	LEU	Х	693	13.479	31.969	41.458	1.00	40.00	6
- 1	20	ATOM	56	CD2	LEU	Х	693	11.884	30.126	41.579		40.00	6
		ATOM	57	С	LEU	Х	693	14.143	28.531	45.054	1.00	40.00	6
		ATOM	58	0	LEU	Х	693	14.702	27.508	44.633	1.00	40.00	8
		ATOM	59	N	LEU	Х	694	14.400	29.079	46.209	1.00	40.00	7
design of the second		ATOM	60	CA	LEU	Х	694	15.407	28.538	47.115		40.00	6
道:	25	ATOM	61	CB	LEU	Х	694	15.871	29.626	48.084		40.00	6
111		ATOM	62	CG	LEU	Х	694	16.692	30.716	47.404		40.00	6
(1)		ATOM	63	CD1	LEU	Х	694	17.279	31.724	48.391		40.00	6
j.sk		ATOM	64	CD2	LEU	Х	694	17.879	30.156	46.619	1.00	40.00	6
1		ATOM	65	С	LEU	Х	694	14.837	27.404	47.957		40.00	6
1186	30	ATOM	66	0	LEU	Х	694	15.555	26.747	48.716		40.00	8
A		ATOM	67	N	GLN	Х	695	13.554	27.157	47.809		40.00	7
21 2004		ATOM	68	CA	GLN	Х	695	12.883	26.188	48.685		40.00	6
507		ATOM	69	C	GLN	Х	695	12.423	24.910	47.977		40.00	6
W		ATOM	70	0	GLN	Х	695	12.309	23.845	48.598		40.00	8
	35	ATOM	71	CB	GLN			11.681	26.858	49.322		40.00	6
10		ATOM	72	CG	GLN	Х	695	12.074	28.125	50.080		20.00	6
vi)		MOTA	73	CD	GLN	Х	695	10.899	28.768	50.801		20.00	6
100		ATOM	74	OE1	GLN	Х	695	9.772	28.296	50.671		20.00	8
		ATOM	75	NE2	GLN			11.092	29.828	51.560		20.00	7
	40	ATOM	76	N	ASP		696	12.155	25.020	46.714		40.00	7
		ATOM	77	CA	ASP			11.698	23.885	45.910		40.00	6
		MOTA	78	CB	ASP			11.450	24.400	44.497		40.00	6
		ATOM	79		ASP			10.782	23.411	43.548		40.00	6
		ATOM	80		ASP			10.550	22.203	43.920		40.00	8
	45	ATOM	81		ASP			10.449	23.804	42.362		40.00	8
		ATOM	82	C	ASP			12.774	22.806	45.876		40.00	6
		MOTA	83		ASP			13.937	23.077	45.562		40.00	8
		ATOM	84		SER			12.370	21.610	46.213		40.00	7
		ATOM	85				697	13.258	20.453	46.128		40.00	6
	50	ATOM	86		SER			12.685	19.371	47.049		40.00	6
		MOTA	87	OG			697	12.535	19.899	48.374		40.00	8
		MOTA	88	С	SER			13.329	20.130	44.613		40.00	6
		ATOM	89	0			697	14.247	20.573	43.914		40.00	8
		ATOM	90		SER			12.355	19.357	44.183		40.00	7
	55	ATOM	91				698	11.985	19.100	42.752		40.00	6
		ATOM	92				698	11.693	20.417	42.036		40.00	6
		ATOM	93				698	10.510	21.000	42.577		40.00	8 6
		ATOM	94	C	SER	Х	698	12.887	18.340	41.758	1.00	40.00	ь

	5	ATOM	95	0	SER	Х	698	13.253	17.158	42.026	1.00	40.00	8
		ATOM	96	OXT	SER	Х	698	13.131	18.976	40.714	1.00	40.00	8
		TER											
		ATOM	1	CB	LYS	Y	688	-33.793	96.885	6.491	1.00	40.00	6
		ATOM	2	С	LYS			-35.002	95.370	8.130	1.00	40.00	6
	10	ATOM	3	ō	LYS			-36.027	95.520	8.779	1.00	40.00	8
	10	ATOM	4	N	LYS		688	-32.717	96.619	8.695	1.00	40.00	7
			5	CA		Y		-34.040	96.591	7.954		40.00	6
		ATOM			ILE			-34.578	93.781	6.908		40.00	7
		ATOM	6	N					93.106	7.268		40.00	6
		ATOM	7	CA			689	-35.862		6.572		40.00	6
	15	ATOM	8	CB	ILE			-35.971	91.759	6.932		40.00	6
		ATOM	9	CG2	ILE			-37.270	91.077			40.00	6
		ATOM	10		ILE		689	-35.917	91.937	5.062			
		ATOM	11	CD1				-36.341	90.691	4.289		40.00	6
		ATOM	12	C	ILE			-36.032	92.870	8.780		40.00	6
	20	ATOM	13	0	ILE			-36.913	93.446	9.442		40.00	8
		ATOM	14	N	LEU	Y	690	-35.019	92.834	9.787		40.00	7
		ATOM	15	CA	LEU	Y	690	-34.956	92.320	11.163		40.00	6
		ATOM	16	CB	LEU	Y	690	-33.528	92.432	11.697		40.00	6
(3		ATOM	17	CG	LEU	Υ	690	-32.516	91.647	10.864		40.00	6
130	25	ATOM	18	CD1	LEU	Y	690	-31.087	91.764	11.397	1.00	40.00	6
11		ATOM	19	CD2	LEU	Y	690	-32.819	90.148	10.812	1.00	40.00	6
10		ATOM	20	С	LEU	Y	690	-35.899	93.123	12.065	1.00	40.00	6
finds		ATOM	21	ō			690	-36.570	92.492	12.928	1.00	40.00	8
N		ATOM	22	N	HIS			-36.039	94.731	11.373	1.00	40.00	7
garb.	30	ATOM	23	CA			691	-36.634	94.923	12.683	1.00	40.00	6
14	50	ATOM	24	CB			691	-36.854	96.383	12.935	1.00	40.00	6
51		ATOM	25	CG			691	-35.610	97.153	13.078		40.00	6
13		ATOM	26		HIS			-34.757	97.640	12.159		40.00	6
1,J			27		HIS			-35.129	97.579	14.319		40.00	7
LU	35	ATOM	28		HIS			-34.039	98.290	14.122		40.00	6
1114	33	ATOM			HIS			-33.786	98.346	12.815		40.00	7
195		ATOM	29				691	-37.972	94.287	12.756		40.00	6
10		ATOM	30	C				-38.240	93.417	13.545		40.00	8
		ATOM	31	0			691	-38.265	94.388	11.505		40.00	7
		ATOM	32	N			692		93.869	11.276		40.00	6
	40	ATOM	33	CA	ARG			-39.577		9.795		40.00	6
		ATOM	34	CB			692	-39.653	93.692 92.764	9.329		40.00	6
		ATOM	35	CG	ARG			-40.759				40.00	6
		MOTA	36	CD	ARG			-40.618	92.422	7.848			7
		MOTA	37	NE			692	-41.849	92.641	7.091		40.00	6
	45	MOTA	38	CZ	ARG			-41.898	92.758	5.763		40.00	
		ATOM	39		ARG			-40.784	92.695	5.024		40.00	7
		ATOM	40	NH2	ARG			-43.034	92.940	5.080		40.00	7
		ATOM	41	C	ARG	Y	692	-39.941	92.547	11.995		40.00	6
		ATOM	42	0	ARG	Y	692	-41.001	92.440	12.649		40.00	8
	50	ATOM	43	N	LEU	Y	693	-39.095	91.576	11.816		40.00	7
		ATOM	44	CA	LEU	Y	693	-39.230	90.232	12.395	1.00	40.00	6
		ATOM	45	CB	LEU	Y	693	-38.362	89.337	11.615	1.00	40.00	6
		ATOM	46	CG	LEU	Y	693	-38.737	89.375	10.132	1.00	40.00	6
		ATOM	47	CD1				-37.794	88.570	9.247	1.00	40.00	6
	55	ATOM	48	CD2			693	-40.142	88.827	9.862	1.00	40.00	6
		ATOM	49	c	LEU			-38.921	90.378	13.816	1.00	40.00	6
		ATOM	50	o	LEU			-39.191	89.474	14.615	1.00	40.00	8
		ATOM	51	N			694	-38.366	91.533	14.076	1.00	40.00	7
		AIOH	51	7.4	0	_	054	55.500					

Atomic Coordinates for Human ER α Complexed with DES, and a GRIP1 NR-box 2 Peptide

	CRYST1	54.09	4 82	. 217	58.	041	90.00	11	1.33 90	.00 P	21	2
10								_	00000			
	ORIGX1		00000	0.000			000000					
	ORIGX2		00000	1.000			000000		00000			
	ORIGX3		00000	0.000			000000		00000			
	SCALE1		18486	0.000			007221		00000			
15	SCALE2		00000	0.012			000000		00000			
	SCALE3	0.0	00000	0.000	0000	0.	018497	0.	00000			
	ATOM	1	CB	SER	A	305			-14.787		1.00	73.26
	ATOM	2	C	SER	A	305			-14.303	1.289	1.00	72.95
20	ATOM	3	0	SER	A	305			-13.984	1.186	1.00	72.46
	MOTA	4	N	SER	A	305			-16.033	0.285	1.00	74.06
	ATOM	5	CA	SER	Α	305			-14.713	0.061	1.00	73.59
	ATOM	6	N	LEU	A	306			-14.313	2.449	1.00	72.21
	ATOM	7	CA	LEU	A	306			-13.950	3.702	1.00	71.05
25	ATOM	8	CB	LEU	A	306			-14.256	4.878	1.00	70.19
-10	ATOM	9	C	LEU	A	306			-12.478	3.719	1.00	69.57
ru	ATOM	10	0	LEU	A	306			-11.638	3.100	1.00	69.96
(O	ATOM	11	N	ALA	A	307			-12.176	4.434	1.00	68.06
Şed:	ATOM	12	CA	ALA	A	307			-10.810	4.541	1.00	64.88
30	ATOM	13	CB	ALA	A	307			-10.795	4.436	1.00	65.83
gents.	ATOM	14	C	ALA	A	307			-10.204	5.866	1.00	63.36
100	ATOM	15	0	ALA	Α	307		.878	-8.984	6.005	1.00	62.73
51	ATOM	16	N	LEU	A	308			-11.062	6.842	1.00	62.52
E	ATOM	17	CA	LEU	A	308			-10.598	8.156	1.00	62.57
14 35	MOTA	18	CB	LEU	A	308		.423	-11.745	9.171	1.00	62.81
الما	ATOM	19	CG	LEU	A	308			-12.688	9.130	1.00	64.21
(5)	ATOM	20	CD1	LEU	Α	308			-13.513		1.00	66.28
10	ATOM	21	CD2	LEU	A	308			-11.898	8.989	1.00	63.80
5	ATOM	22	C	LEU	A	308		.903	-10.037	8.100	1.00	61.61
40	ATOM	23	0	LEU	A	308		.385	-9.445	9.066	1.00	62.92
	MOTA	24	N	SER	A	309		.561		6.959	1.00	60.50
	ATOM	25	CA	SER	A	309		.928	-9.743	6.771	1.00	58.73
	ATOM	26	CB	SER	A	309		.720	-10.750	5.934	1.00	59.53
	ATOM	27	OG	SER	Α	309		8.889		4.606	1.00	59.47
45	ATOM	28	C	SER	A	309		7.986	-8.373	6.099	1.00	57.05
	ATOM	29	0	SER	A	309		3.965	-7.637	6.249	1.00	56.70
	ATOM	30	N	LEU	A	310		.940	-8.038	5.352	1.00	52.69
	ATOM	31	CA	LEU	A	310		.877	-6.759	4.658	1.00	48.20
	ATOM	32	CB	LEU	A	310	3.5	5.516	-6.596	3.974	1.00	48.32
50	ATOM	33	CG	LEU	A	310	35	5.301		2.583	1.00	
	ATOM	34	CD1	LEU	A	310	33	3.951		2.055	1.00	
	ATOM	35	CD2	LEU	A	310	3 (5.417	-6.755	1.650	1.00	
	ATOM	36	C	LEU	A	310	3"	7.086	-5.589	5.609	1.00	
	ATOM	37	0	LEU	A	310	3 (5.605		6.741	1.00	
55	ATOM	38	N	THR	A	311	. 31	7.812	-4.576	5.148	1.00	
33	ATOM	39	CA	THR	A	311	. 31	3.034	-3.380	5.949	1.00	
	MOTA	40	CB	THR	A	311		9.313	-2.633		1.00	
	ATOM	41	OG1	THR	A	311		9.079	-1.936		1.00	
	MOTA	42	CG2	THR	A	311		0.464		5.350	1.00	
60	ATOM	43	C	THR	A	311		6.834	-2.475		1.00	
30	ATOM	44	0	THR	A	311		6.021	-2.776	4.800	1.00	42.12
	AT OLI		-									

	5	ATOM	45	N	ALA	A	312	36.726	-1.372	6.409	1.00	42.16
	,	ATOM	46	CA	ALA	A	312	35.616	-0.444	6.228	1.00	40.10
		ATOM	47	CB	ALA	A	312	35.741	0.709	7.205	1.00	40.07
			48	C	ALA	A	312	35.561	0.090	4.799	1.00	41.80
		ATOM	49	0	ALA	A	312	34.510	0.074	4.154	1.00	37.81
	10	ATOM	50	N	ASP	A	313	36.698	0.564	4.304	1.00	42.35
	10	MOTA			ASP	A	313	36.752	1.104	2.953	1.00	42.27
		ATOM	51	CA CB	ASP	A	313	38.133	1.703	2.680	1.00	43.74
		MOTA	52		ASP	A	313	38.323	3.054	3.348	1.00	46.62
		MOTA	53	CG		A	313	39.414	3.645	3.205	1.00	51.01
		ATOM	54	OD1	ASP			37.380	3.529	4.015	1.00	48.89
	15	MOTA	55	OD2	ASP	A	313	36.422	0.027	1.926	1.00	38.68
		ATOM	56	C	ASP	A	313	35.704	0.281	0.959	1.00	38.75
		ATOM	57	0	ASP	A	313		-1.179	2.145	1.00	34.76
		MOTA	58	N	GLN	A	314	36.931	-2.277	1.229	1.00	33.55
		ATOM	59	CA	GLN	Α	314	36.666			1.00	36.90
	20	MOTA	60	CB	GLN	A	314	37.462	-3.512	1.643	1.00	40.45
		MOTA	61	CG	GLN	A	314	38.963	-3.384			43.13
		ATOM	62	CD	GLN	Α	314	39.700	-4.610	1.905	1.00	
		ATOM	63	OE1	GLN	A	314	39.394	-5.196	2.935	1.00	43.60
		ATOM	64	NE2	GLN	A	314	40.701	-5.032	1.117	1.00	44.03
(2)	25	ATOM	65	C	GLN	A	314	35.176	-2.595	1.201	1.00	34.95
10		ATOM	66	0	GLN	Α	314	34.605	-2.860	0.140	1.00	32.89
fu		MOTA	67	N	MET	Α	315	34.542	-2.564	2.374	1.00	32.54
(1)		ATOM	68	CA	MET	A	315	33.115	-2.848	2.470	1.00	35.46
- Bak		ATOM	69	CB	MET	A	315	32.650	-2.794	3.926	1.00	37.09
1	30	ATOM	70	CG	MET	A	315	31.137	-2.777	4.097	1.00	39.42
- Long		MOTA	71	SD	MET	A	315	30.443	-4.426	4.053	1.00	46.55
34		ATOM	72	CE	MET	A	315	31.351	-5.205	5.397	1.00	45.29
8		ATOM	73	C	MET	A	315	32.311	-1.859	1.640	1.00	31.83
		ATOM	74	0	MET	A	315	31.453	-2.247	0.852	1.00	32.10
	35	MOTA	75	N	VAL	A	316	32.587	-0.560	1.830	1.00	32.62
8.4		ATOM	76	CA	VAL	Α	316	31.882	0.470	1.079	1.00	31.09
		ATOM	77	CB	VAL	A	316	32.395	1.888	1.425	1.00	34.77
ıÜ.		ATOM	78	CG1	VAL	Α	316	31.786	2.899	0.461	1.00	34.10
		ATOM	79	CG2	VAL	A	316	32.021	2.246	2.862	1.00	34.40
-5	40	ATOM	80	C	VAL	A	316	32.092	0.232	-0.414	1.00	33.48
		ATOM	81	0	VAL	A	316	31.145		-1.200	1.00	32.49
		ATOM	82	N	SER	A	317	33.337	-0.027	-0.795	1.00	33.49
		ATOM	83	CA	SER	A	317	33.682	-0.280	-2.187	1.00	32.88
		ATOM	84	CB	SER	A	317	35.165	-0.635	-2.297	1.00	35.77
	45	MOTA	85	OG	SER	A	317	35.825	0.277	-3.154	1.00	42.70
	15	ATOM	86	C	SER	Α	317	32.849	-1.396	-2.801	1.00	30.71
		ATOM	87	Ö	SER	A	317	32.279	-1.238	-3.880	1.00	31.14
		ATOM	88	N	ALA	A	318	32.792	-2.529	-2.111	1.00	29.51
		ATOM	89	CA	ALA	A	318	32.035		-2.580	1.00	29.93
	50		90	CB	ALA	A	318	32.156		-1.579	1.00	28.56
	30	ATOM	91	C	ALA	A	318	30.565		-2.771	1.00	31.55
		MOTA	92	0	ALA	A	318	29.961		-3.784	1.00	30.64
		MOTA		N	LEU	A	319	29.997		-1.791	1.00	34.13
		ATOM	93			A	319	28.597		-1.861	1.00	32.93
		ATOM	94	CA	LEU	A	319	28.170		-0.540	1.00	31.15
	55	MOTA	95	CB				28.076	-2.555		1.00	32.27
		MOTA	96	CG	LEU	A	319	27.523	-1.840	1.852	1.00	32.14
		MOTA	97	CD1	LEU	A	319	27.523	-3.733		1.00	31.82
		MOTA	98	CD2	LEU	A	319	28.340		-3.020	1.00	34.41
		MOTA	99	C	LEU	A	319	28.340		-3.818	1.00	35.23
	60	MOTA	100	0	LEU	A	319			-3.120	1.00	32.53
		ATOM	101	N	LEU	A	320	29.140		-4.212	1.00	35.33
		MOTA	102	CA	LEU	A	320	28.972	0.750	-4.212	1.00	55.55

	5	ATOM	103	CB	LEU	Α	320	30.052	1.839 -4.155	1.00	33.52
		ATOM	104	CG	LEU	A	320	29.974	2.899 -3.054	1.00	34.60
		MOTA	105	CD1	LEU	Α	320	31.060	3.940 -3.292	1.00	33.69
		ATOM	106	CD2	LEU	A	320	28.611	3.562 -3.044	1.00	31.05
		MOTA	107	C	LEU	Α	320	29.052	0.040 -5.561	1.00	35.41
	10	ATOM	108	0	LEU	Α	320	28.230	0.271 -6.446	1.00	39.16
		ATOM	109	N	AASP	Α	321	30.042	-0.833 -5.720	0.50	36.33
		ATOM	110	N	BASP	A	321	30.041	-0.839 -5.695	0.50	35.76
		ATOM	111	CA	AASP	A	321	30.214	-1.559 -6.977	0.50	37.71
		ATOM	112	CA	BASP	A	321	30.258	-1.595 -6.925	0.50	37.11
	15	ATOM	113	CB	AASP	A	321	31.537	-2.334 -6.973	0.50	40.01
	15	ATOM	114	CB	BASP	A	321	31.573	-2.374 -6.826	0.50	39.41
		ATOM	115	CG	AASP	A	321	31.694	-3.230 -8.195	0.50	41.93
		ATOM	116	CG	BASP	A	321	32.770	-1.562 -7.284	0.50	39.96
	20	ATOM	117	OD1	AASP	A	321	31.523	-2.733 -9.329	0.50	42.11
	20	ATOM	118	OD1	BASP	A	321	33.312	-1.868 -8.366	0.50	43.41
		ATOM	119	OD2	AASP	A	321	31.988	-4.432 -8.022	0.50	42.69
		ATOM	120	OD2	BASP	Α	321	33.170	-0.622 -6.564	0.50	41.33
		ATOM	121	C	AASP	Α	321	29.069	-2.524 -7.275	0.50	37.19
		ATOM	122	C	BASP	А	321	29.123	-2.565 -7.253	0.50	36.68
	25	ATOM	123	0	AASP	Α	321	28.820	-2.861 -8.434	0.50	36.87
Ū		ATOM	124	0	BASP	А	321	28.934	-2.942 -8.411	0.50	36.08
U		ATOM	125	N	ALA	А	322	28.374	-2.968 -6.235	1.00	35.35
Ü		ATOM	126	CA	ALA	A	322	27.268	-3.902 -6.417	1.00	31.59
ı dir		ATOM	127	CB	ALA	А	322	27.124	-4.781 -5.175	1.00	30.73
154	30	ATOM	128	C	ALA	Α	322	25.946	-3.204 -6.709	1.00	30.07
nist		ATOM	129	0	ALA	Α	322	24.955	-3.857 -7.036	1.00	26.53
1		ATOM	130	N	GLU	Α	323	25.932	-1.880 -6.596	1.00	27.98
i i		ATOM	131	CA	GLU	Α	323	24.713	-1.117 -6.827	1.00	29.88
106		ATOM	132	CB	GLU	Α	323	25.027	0.380 -6.855	1.00	30.98
1	35	ATOM	133	CG	GLU	Α	323	24.870	1.068 -5.509	1.00	31.62
11		ATOM	134	CD	GLU	Α	323	23.463	0.940 -4.960	1.00	31.98
7		ATOM	135	OE1	GLU	Α	323	23.183	-0.056 -4.257	1.00	33.10
75		ATOM	136	OE2	GLU	Α	323	22.640	1.836 -5.233	1.00	30.01
Ö		ATOM	137	C	GLU	A	323	24.010	-1.515 -8.123	1.00	30.86
Serv	40	ATOM	138	0	GLU	Α	323	24.655	-1.705 -9.151	1.00	28.86
		ATOM	139	N	PRO	Α	324	22.674	-1.659 -8.083	1.00	30.66
		ATOM	140	CD	PRO	A	324	21.774	-1.466 -6.935	1.00	31.01
		ATOM	141	CA	PRO	A	324	21.935	-2.032 -9.290	1.00	30.29
		ATOM	142	CB	PRO	Α	324	20.613	-2.598 -8.760	1.00	31.42
	45	ATOM	143	CG	PRO	Α	324	20.626	-2.363 -7.258	1.00	33.66
		ATOM	144	C	PRO	Α	324	21.717	-0.785-10.138	1.00	27.46
		ATOM	145	0	PRO	Α	324	21.893	0.332 -9.668	1.00	26.19
		ATOM	146	N	PRO	А	325	21.335	-0.959-11.403	1.00	27.80
		ATOM	147	CD	PRO	Α	325	21.082	-2.198-12.161	1.00	27.35
	50	ATOM	148	CA	PRO	A	325	21.125	0.242-12.211	1.00	25.59
	-	ATOM	149	CB	PRO	A	325	21.258	-0.266-13.637	1.00	24.02
		ATOM	150	CG	PRO	A	325	20.773	-1.695-13.559	1.00	26.00
		ATOM	151	C	PRO	A	325	19.749	0.830-11.954	1.00	23.73
		ATOM	152	0	PRO	A	325	18.873	0.165-11.402	1.00	24.83
	55	ATOM	153	N	ILE	A	326	19.571	2.081-12.352	1.00	22.11
	55	ATOM	154	CA	ILE	A	326	18.296	2.762-12.212	1.00	24.01
				CB		A		18.296	4.282-12.133	1.00	25.97
		ATOM	155		ILE	A	326		4.282-12.133	1.00	25.97
		ATOM	156	CG2	ILE	A	326 326	17.168 19.189	4.632-12.286	1.00	29.31
	60	ATOM	157	CG1		A			6.120-10.525	1.00	32.91
	30	ATOM	158		ILE	A	326 326	19.301 17.506	2.408-13.471	1.00	25.72
		ATOM	159	C		A					25.72
		ATOM	160	J	ILE	А	326	17.906	2.758-14.581	1.00	45.55
								152			

	5	ATOM	161	N	LEU	A	327	16.392	1.703-13.301	1.00	25.57
	3	ATOM	162	CA	LEU	A	327	15.595	1.279-14.439	1.00	23.80
		ATOM	163	CB	LEU	A	327	14.872	-0.029-14.104	1.00	23.96
		ATOM	164	CG	LEU	A	327	15.778	-1.210-13.728	1.00	19.89
		ATOM	165	CD1	LEU	A	327	14.944	-2.462-13.583	1.00	21.19
	10	ATOM	166	CD2	LEU	A	327	16.850	-1.415-14.805	1.00	17.53
	10	ATOM	167	C	LEU	A	327	14.598	2.317-14.935	1.00	27.16
			168	0	LEU	A	327	14.161	3.202-14.194	1.00	25.98
		ATOM		N	TYR	A	328	14.251	2.207-16.210	1.00	26.56
		ATOM	169		TYR	A	328	13.303	3.123-16.814	1.00	24.45
		ATOM	170	CA		A	328	13.724	3.465-18.245	1.00	26.72
	15	ATOM	171	CB	TYR		328	14.587	4.693-18.314	1.00	27.73
		MOTA	172	CG	TYR	A		14.021	5.949-18.518	1.00	28.56
		ATOM	173	CD1	TYR	A	328		7.092-18.509	1.00	29.10
		MOTA	174	CE1	TYR	A	328	14.798	4.612-18.110	1.00	26.01
		MOTA	175	CD2	TYR	A	328	15.962	5.753-18.098	1.00	30.63
	20	ATOM	176	CE2	TYR	A	328	16.750	6.988-18.297	1.00	30.07
		MOTA	177	CZ	TYR	A	328	16.157		1.00	37.94
		MOTA	178	OH	TYR	A	328	16.917	8.130-18.265		24.95
		MOTA	179	C	TYR	A	328	11.923	2.501-16.827	1.00	27.02
		ATOM	180	0	TYR	A	328	11.774	1.274-16.846	1.00	25.60
17	25	MOTA	181	N	SER	A	329	10.912	3.358-16.800	1.00	
10		ATOM	182	CA	SER	A	329	9.533	2.908-16.837	1.00	29.45
T.		MOTA	183	CB	SER	A	329	8.661	3.858-16.020	1.00	30.80
ŧØ.		ATOM	184	OG	SER	A	329	7.297	3.721-16.364	1.00	33.74
feli		ATOM	185	C	SER	A	329	9.129	2.947-18.313	1.00	31.30
4.1	30	ATOM	186	0	SER	Α	329	9.908	3.397-19.154	1.00	27.35
11000		ATOM	187	N	GLU	A	330	7.930	2.469-18.629	1.00	32.98
14		ATOM	188	CA	GLU	A	330	7.459	2.482-20.007	1.00	35.10
8		ATOM	189	CB	GLU	A	330	6.031	1.968-20.074	1.00	34.67
		ATOM	190	C	GLU	A	330	7.532	3.924-20.505	1.00	40.06
(L)	35	MOTA	191	0	GLU	A	330	7.068	4.841-19.826	1.00	42.65
LU		ATOM	192	N	TYR	A	331	8.124	4.126-21.681	1.00	41.16
(10)		ATOM	193	CA	TYR	Α	331	8.263	5.470-22.234	1.00	42.66
lind Lil		ATOM	194	CB	TYR	A	331	9.323	5.482-23.350	1.00	42.54
		ATOM	195	CG	TYR	A	331	9.202	4.347-24.345	1.00	38.67
Q	40	ATOM	196	CD1	TYR	Α	331	10.105	3.284-24.334	1.00	34.66
		ATOM	197	CE1	TYR	Α	331	9.985	2.228-25.233	1.00	34.89
		ATOM	198	CD2	TYR	Α	331	8.174	4.327-25.287	1.00	37.88
		ATOM	199	CE2	TYR	A	331	8.045	3.276-26.193	1.00	34.65
		ATOM	200	CZ	TYR	A	331	8.950	2.232-26.159	1.00	30.73
	45	ATOM	201	OH	TYR	A	331	8.814	1.191-27.042	1.00	30.97
	43	ATOM	202	C	TYR	A	331	6.943	6.043-22.754	1.00	46.24
		ATOM	203	0	TYR	A	331	6.018	5.301-23.096	1.00	45.38
		ATOM	204	N	ASP	A	332	6.868	7.372-22.792	1.00	49.11
			205	CA	ASP	A	332	5.684	8.092-23.262	1.00	52.40
	50	ATOM	205	CB	ASP	A	332	5.781	8.321-24.772	1.00	52.86
	30	MOTA		C	ASP	A	332	4.356	7.410-22.926	1.00	52.90
		MOTA	207	0	ASP	A	332	3.561	7.116-23.818	1.00	53.94
		ATOM	208		PRO	A	333	4.103	7.144-21.632	1.00	53.63
		MOTA	209	N		A	333	4.962	7.418-20.465	1.00	53.63
		ATOM	210	CD	PRO		333	2.840	6.497-21.253	1.00	53.55
	55	MOTA	211	CA	PRO	A		3.070	6.076-19.802	1.00	53.78
		MOTA	212	CB	PRO	A	333	4.101	7.028-19.290	1.00	53.42
		MOTA	213	CG	PRO	A	333	1.673	7.478-21.398	1.00	52.17
		MOTA	214	C	PRO	A	333	1.673	8.690-21.395	1.00	51.19
		ATOM	215	0	PRO	A	333		6.956-21.532	1.00	52.26
	60	ATOM	216	N	THR	A	334	0.457	7.802-21.687	1.00	54.21
		MOTA	217	CA	THR	A	334	-0.724	6.949-21.813	1.00	53.90
		MOTA	218	CB	THR	A	334	-1.997	0.747-21.013	1.00	55.50

								5 055 03 0CF	1.00	53.92
5	MOTA	219	OG1	THR	Α	334	-1.971			
	MOTA	220	CG2	THR	A	334	-3.237		1.00	54.15
	ATOM	221	C	THR	Α	334	-0.864		1.00	56.34
	ATOM	222	0	THR	A	334	-1.389	8.443-19.461	1.00	56.44
	ATOM	223	N	ARG	Α	335	-0.386	10.002-20.766	1.00	58.24
10	ATOM	224	CA	ARG	Α	335	-0.377	11.099-19.801	1.00	57.96
10	ATOM	225	CB	ARG	A	335	-0.569	12.427-20.531	1.00	60.22
		226	C	ARG	A	335	-1.349	10.996-18.627	1.00	56.61
	MOTA			ARG	A	335	-0.919	10.908-17.475	1.00	60.70
	MOTA	227	0		A	336	-2.667	11.015-18.889	1.00	52.43
	MOTA	228	N	PRO			-3.389	11.117-20.165	1.00	49.06
15	MOTA	229	CD	PRO	A	336		10.915-17.752	1.00	49.58
	MOTA	230	CA	PRO	A	336	-3.587		1.00	48.66
	MOTA	231	CB	PRO	A	336	-4.911	11.456-18.302		51.33
	ATOM	232	CG	PRO	Α	336	-4.645	11.809-19.760	1.00	
	ATOM	233	C	PRO	Α	336	-3.698	9.468-17.279	1.00	49.25
20	ATOM	234	0	PRO	A	336	-4.340	8.644-17.929	1.00	48.06
	ATOM	235	N	PHE	A	337	-3.063	9.170-16.147	1.00	47.90
	ATOM	236	CA	PHE	A	337	-3.055	7.821-15.582	1.00	46.61
	ATOM	237	CB	PHE	Α	337	-2.063	7.732-14.421	1.00	47.73
	ATOM	238	CG	PHE	A	337	-0.649	8.011-14.805	1.00	46.27
11 25	ATOM	239	CD1	PHE	A	337	-0.017	9.168-14.368	1.00	46.55
1112			CD2	PHE	A	337	0.061	7.113-15.591	1.00	48.12
103	MOTA	240	CE1	PHE	A	337	1.305	9.429-14.707	1.00	48.09
17.2	MOTA	241		PHE	A	337	1.386	7.364-15.938	1.00	47.57
100	ATOM	242	CE2				2.009	8.525-15.495	1.00	48.40
air	ATOM	243	CZ	PHE	A	337		7.338-15.071	1.00	46.15
30	ATOM	244	C	PHE	Α	337	-4.401		1.00	48.34
forth.	MOTA	245	0	PHE	A	337	-5.250	8.127-14.671		45.06
344	MOTA	246	N	SER	A	338	-4.573	6.022-15.080	1.00	
50	ATOM	247	CA	SER	A	338	-5.781	5.385-14.578	1.00	45.12
0	MOTA	248	CB	SER	A	338	-6.477	4.594-15.684	1.00	44.49
35	ATOM	249	OG	SER	Α	338	-6.227	3.206-15.554	1.00	45.78
L.	MOTA	250	C	SER	A	338	-5.292	4.439-13.488	1.00	47.04
1200	MOTA	251	0	SER	Α	338	-4.090	4.186-13.387	1.00	44.08
(25) an	MOTA	252	N	GLU	A	339	-6.206	3.916-12.676	1.00	45.63
-D	MOTA	253	CA	GLU	A	339	-5.802	3.012-11.608	1.00	45.40
₽ 40	ATOM	254	CB	GLU	Α	339	-7.015	2.521-10.814	1.00	45.66
40	ATOM	255	CG	GLU	A	339	-6.637	1.680 -9.600	1.00	46.81
		256	CD	GLU	A	339	-7.717	1.652 -8.535	1.00	47.56
	ATOM		OE1	GLU	A	339	-8.471	0.656 -8.477	1.00	47.37
	ATOM	257	OE2	GLU	A	339	-7.810	2.625 -7.754	1.00	49.29
	ATOM	258				339	-5.040	1.821-12.170	1.00	45.23
45	MOTA	259	C	GLU	A		-3.862	1.641-11.872	1.00	46.51
	ATOM	260	0	GLU	A	339	-5.712	1.010-12.982	1.00	42.87
	MOTA	261	N	ALA	A	340		-0.158-13.574	1.00	40.24
	ATOM	262	CA	ALA	A	340	-5.078		1.00	41.40
	ATOM	263	CB	ALA	A	340	-6.055	-0.871-14.496		38.83
50	MOTA	264	C	ALA	A	340	-3.837	0.273-14.350	1.00	
	ATOM	265	0	ALA	A	340	-2.909	-0.515-14.543	1.00	35.58
	ATOM	266	N	SER	Α	341	-3.836	1.535-14.773	1.00	35.79
	MOTA	267	CA	SER	A	341	-2.742	2.133-15.537	1.00	36.58
	MOTA	268	CB	SER	A	341	-3.231	3.454-16.154	1.00	39.01
55	ATOM	269	OG	SER	A	341	-2.211	4.130-16.864	1.00	36.09
33	ATOM	270	C	SER	A	341	-1.480	2.376-14.691	1.00	35.63
		271	0	SER	A	341	-0.389	1.913-15.038	1.00	33.20
	MOTA		N	MET	A	342	-1.626	3.115-13.595	1.00	35.92
	MOTA	272			A	342	-0.498	3.396-12.708	1.00	35.88
	ATOM	273	CA	MET		342	-0.438	4.396-11.623	1.00	35.96
60	ATOM	274	CB	MET	A			5.218-11.059	1.00	38.02
	MOTA	275	CG	MET	A	342	0.241	6.374 -9.780	1.00	44.73
	ATOM	276	SD	MET	A	342	-0.308	0.3/4 -9./80	1.00	11./3

										1 00	42.49
	5	ATOM	277	CE	MET	A	342	0.626	7.815-10.205	1.00	
		ATOM	278	C	MET	A	342	-0.011	2.100-12.059	1.00	34.17
		ATOM	279	0	MET	A	342	1.195	1.880-11.909	1.00	33.40
		ATOM	280	N	MET	A	343	-0.957	1.243-11.687	1.00	29.95
		ATOM	281	CA	MET	A	343	-0.640	-0.034-11.062	1.00	31.96
	10		282	CB	MET	A	343	-1.921	-0.810-10.751	1.00	31.70
	10	ATOM					343	-2.667	-0.337 -9.502	1.00	37.13
		MOTA	283	CG	MET	A		-1.749	-0.507 -7.940	1.00	36.00
		ATOM	284	SD	MET	A	343			1.00	32.14
		ATOM	285	CE	MET	A	343	-1.468	-2.299 -7.886		
		ATOM	286	C	MET	Α	343	0.234	-0.875-11.979	1.00	31.72
	15	ATOM	287	0	MET	A	343	1.159	-1.558-11.527	1.00	30.26
		ATOM	288	N	GLY	A	344	-0.069	-0.823-13.272	1.00	29.04
		ATOM	289	CA	GLY	Α	344	0.688	-1.591-14.242	1.00	24.94
		ATOM	290	C	GLY	Α	344	2.104	-1.085-14.396	1.00	26.01
		ATOM	291	0	GLY	A	344	3.046	-1.873-14.463	1.00	28.72
	20				LEU	A	345	2.257	0.232-14.471	1.00	26.97
	20	ATOM	292	N			345	3.576	0.839-14.608	1.00	31.15
		ATOM	293	CA	LEU	A		3.459	2.361-14.753	1.00	30.06
		ATOM	294	CB	LEU	A	345		2.924-15.995	1.00	33.50
		MOTA	295	CG	LEU	A	345	2.765			33.50
		ATOM	296	CD1	LEU	Α	345	2.901	4.439-15.999	1.00	
120	25	ATOM	297	CD2	LEU	A	345	3.379	2.324-17.257	1.00	33.22
10		ATOM	298	C	LEU	A	345	4.433	0.534-13.383	1.00	30.31
ïÜ		ATOM	299	0	LEU	A	345	5.564	0.061-13.505	1.00	32.80
173		ATOM	300	N	LEU	A	346	3.884	0.813-12.205	1.00	27.83
lake lake		ATOM	301	CA	LEU	Α	346	4.595	0.596-10.947	1.00	26.19
1	30	ATOM	302	CB	LEU	A	346	3.729	1.063 -9.783	1.00	24.51
	30	ATOM	303	CG	LEU	A	346	3.483	2.569 -9.682	1.00	26.33
godi.				CD1	LEU	A	346	2.623	2.844 -8.463	1.00	27.33
14		ATOM	304			A	346	4.809	3.317 -9.587	1.00	24.89
69		MOTA	305	CD2	LEU			5.032	-0.848-10.707	1.00	25.72
1200		ATOM	306	C	LEU	A	346		-1.102-10.345	1.00	29.86
Li	35	ATOM	307	0	LEU	A	346	6.181		1.00	23.80
1,1		MOTA	308	N	THR	A	347	4.117	-1.793-10.891		23.91
1204		ATOM	309	CA	THR	A	347	4.436	-3.196-10.674	1.00	
10		ATOM	310	CB	THR	Α	347	3.164	-4.058-10.641	1.00	26.39
		ATOM	311	OG1	THR	A	347	2.421	-3.860-11.849	1.00	24.57
12.2	40	ATOM	312	CG2	THR	A	347	2.301	-3.682 -9.444	1.00	23.98
		ATOM	313	C	THR	A	347	5.366	-3.734-11.756	1.00	26.17
		ATOM	314	0	THR	Α	347	6.176	-4.622-11.496	1.00	27.44
		ATOM	315	N	ASN	Α	348	5.242	-3.197-12.970	1.00	25.48
		ATOM	316	CA	ASN	A	348	6.092	-3.617-14.082	1.00	23.77
	45	ATOM	317	CB	ASN	A	348	5.657	-2.926-15.385	1.00	24.59
	45		318	CG	ASN	A	348	6.522	-3.302-16.571	1.00	29.93
		ATOM				A	348	7.616	-2.799-16.771	1.00	24.81
		MOTA	319	OD1	ASN			6.010	-4.236-17.391	1.00	32.61
		MOTA	320	ND2	ASN	A	348		-3.229-13.741	1.00	22.82
		ATOM	321	C	ASN	A	348	7.532			18.83
	50	ATOM	322	0	ASN	Α	348	8.453	-4.027-13.870	1.00	
		ATOM	323	N	LEU	A	349	7.711	-1.993-13.288	1.00	22.58
		ATOM	324	CA	LEU	A	349	9.030	-1.507-12.914	1.00	21.85
		ATOM	325	CB	LEU	A	349	8.929	-0.028-12.536	1.00	22.00
		ATOM	326	CG	LEU	Α	349	10.155	0.673-11.953	1.00	23.64
	55	ATOM	327	CD1	LEU	Α	349	11.224	0.826-13.017	1.00	19.35
	55		328	CD2	LEU	A	349	9.726	2.040-11.415	1.00	21.97
		ATOM		CDZ	LEU	A	349	9.564	-2.335-11.734	1.00	22.94
		ATOM	329					10.724	-2.749-11.717	1.00	23.97
		MOTA	330	0	LEU	A	349 350	8.705	-2.591-10.756	1.00	21.67
		MOTA	331	N	ALA	A			-3.356 -9.586	1.00	21.83
	60	MOTA	332	CA	ALA	A	350	9.113		1.00	18.95
		MOTA	333	CB	ALA	A	350	7.963	-3.441 -8.593		21.90
		ATOM	334	C	ALA	Α	350	9.568	-4.757 -9.985	1.00	21.50

	5	ATOM	335	0	ALA	A	350	10.625	-5.221 -9.554	1.00	24.15
	,	ATOM	336	N	ASP	А	351	8.767	-5.423-10.810	1.00	23.24
		ATOM	337	CA	ASP	A	351	9.093	-6.772-11.259	1.00	25.87
			338	CB	ASP	A	351	8.028	-7.274-12.239	1.00	27.03
		MOTA		CG	ASP	A	351	8.103		1.00	31.64
	10	MOTA	339		ASP	A	351	8.217		1.00	35.06
	10	ATOM	340	OD1				8.049	-9.525-11.464	1.00	36.86
		MOTA	341	OD2	ASP	A	351		-6.825-11.912	1.00	22.36
		MOTA	342	C	ASP	A	351	10.469	-7.773-11.702	1.00	25.15
		ATOM	343	0	ASP	A	351	11.219			23.58
		ATOM	344	N	ARG	Α	352	10.810	-5.808-12.697	1.00	
	15	ATOM	345	CA	ARG	A	352	12.115	-5.787-13.347	1.00	21.07
		ATOM	346	CB	ARG	Α	352	12.120	-4.785-14.507	1.00	21.02
		ATOM	347	CG	ARG	A	352	11.539	-5.352-15.797	1.00	20.44
		ATOM	348	CD	ARG	A	352	11.554	-4.319-16.915	1.00	20.43
		ATOM	349	NE	ARG	A	352	10.592	-3.245-16.687	1.00	19.85
	20	ATOM	350	CZ	ARG	A	352	10.910	-1.954-16.641	1.00	19.69
		ATOM	351	NH1	ARG	А	352	12.172	-1.564-16.813	1.00	17.36
		ATOM	352	NH2	ARG	Α	352	9.962	-1.049-16.441	1.00	21.88
		ATOM	353	C	ARG	A	352	13.223	-5.442-12.350	1.00	22.11
			354	0	ARG	A	352	14.346	-5.945-12.454	1.00	24.13
	25	ATOM	355	N	GLU	A	353	12.909	-4.587-11.383	1.00	18.66
Con Cons	25	ATOM				A	353	13.888	-4.206-10.376	1.00	19.08
157		MOTA	356	CA	GLU			13.317	-3.102 -9.483	1.00	21.62
10		MOTA	357	CB	GLU	A	353	13.295	-1.718-10.114	1.00	20.97
10		ATOM	358	CG	GLU	A	353		-0.648 -9.129	1.00	23.84
g mais		MOTA	359	CD	GLU	Α	353	12.832		1.00	24.76
123	30	ATOM	360	OE1	GLU	Α	353	11.611	-0.531 -8.926		24.70
1.de		MOTA	361	OE2	GLU	A	353	13.686	0.066 -8.557	1.00	20.14
34		MOTA	362	C	GLU	A	353	14.246	-5.423 -9.512	1.00	
		ATOM	363	0	GLU	Α	353	15.398	-5.600 -9.104	1.00	19.40
100		MOTA	364	N	LEU	A	354	13.246	-6.257 -9.235	1.00	19.54
W	35	ATOM	365	CA	LEU	A	354	13.434	-7.452 -8.415	1.00	21.77
1,0		ATOM	366	CB	LEU	A	354	12.107	-8.209 -8.270	1.00	23.09
		ATOM	367	CG	LEU	A	354	11.160	-7.606 -7.223	1.00	25.00
10		ATOM	368	CD1	LEU	Α	354	9.720	-8.013 -7.510	1.00	23.49
		ATOM	369	CD2	LEU	A	354	11.584	-8.069 -5.839	1.00	23.31
133	40	ATOM	370	C	LEU	A	354	14.500	-8.386 -8.981	1.00	23.21
	-10	ATOM	371	ō	LEU	А	354	15.255	-9.007 -8.234	1.00	22.44
		ATOM	372	N	VAL	A	355	14.560	-8.490-10.302	1.00	22.52
		ATOM	373	CA	VAL	A	355	15.551	-9.343-10.935	1.00	21.66
			374	CB	VAL	A	355	15.353	-9.365-12.466	1.00	24.35
	45	MOTA		CG1	VAL	A	355	16.435	-10.214-13.119	1.00	28.16
	43	MOTA	375	CG2	VAL	A	355	13.957	-9.886-12.798	1.00	21.59
		ATOM	376				355	16.944	-8.811-10.606	1.00	23.74
		MOTA	377	C	VAL	A		17.857	-9.581-10.291	1.00	23.51
		MOTA	378	0	VAL	A	355	17.105	-7.489-10.669	1.00	21.27
		MOTA	379	N	HIS	A	356			1.00	21.31
	50	MOTA	380	CA	HIS	A	356	18.392	-6.861-10.369	1.00	19.87
		ATOM	381	CB	HIS	A	356	18.384	-5.390-10.811		21.77
		ATOM	382	CG	HIS	Α	356	18.494	-5.205-12.295	1.00	
		MOTA	383	CD2	HIS	Α	356	17.543	-5.048-13.248	1.00	21.66
		ATOM	384	ND1	HIS	Α	356	19.704	-5.177-12.955	1.00	21.11
	55	ATOM	385	CE1	HIS	A	356	19.496	-5.011-14.249	1.00	24.96
		ATOM	386	NE2	HIS	A	356	18.192	-4.931-14.455	1.00	18.37
		ATOM	387	C	HIS	Α	356	18.702	-6.947 -8.875	1.00	21.41
		ATOM	388	ō	HIS	A	356	19.864	-7.111 -8.465	1.00	21.88
		ATOM	389	N	MET	A	357	17.660	-6.843 -8.058	1.00	21.84
	60	ATOM	390	CA	MET	A	357	17.837	-6.906 -6.610	1.00	21.51
	00	ATOM	391	CB	MET	A	357	16.503	-6.668 -5.898	1.00	17.60
		ATOM	392	CG	MET	A	357	16.629	-6.579 -4.369	1.00	19.36
		AIOM	3,2					156			

						_		15.051 -6.755 -3.531 1.00 23.64
	5	MOTA	393	SD	MET	A	357	
		ATOM	394	CE	MET	Α	357	
		ATOM	395	C	MET	A	357	18.411 -8.259 -6.192 1.00 23.69
		ATOM	396	0	MET	A	357	19.337 -8.328 -5.389 1.00 24.41
		ATOM	397	N	ILE	Α	358	17.856 -9.331 -6.746 1.00 27.14
	10	ATOM	398	CA	ILE	A	358	18.314 -10.672 -6.425 1.00 28.79
	10	ATOM	399	CB	ILE	A	358	17.529 -11.725 -7.232 1.00 32.42
			400	CG2	ILE	A	358	18.267 -13.064 -7.220 1.00 32.77
		MOTA			ILE	A	358	16.125 -11.880 -6.644 1.00 31.94
		ATOM	401	CG1			358	15.062 -12.196 -7.680 1.00 34.85
		MOTA	402	CD1	ILE	A		19.801 -10.802 -6.728 1.00 28.75
	15	MOTA	403	C	ILE	A	358	13.001 10.001
		MOTA	404	0	ILE	A	358	20.000
		ATOM	405	N	ASN	A	359	
		ATOM	406	CA	ASN	A	359	21.601 -10.401 -8.293 1.00 29.16
		ATOM	407	CB	ASN	A	359	21.721 -10.172 -9.801 1.00 31.88
	20	ATOM	408	CG	ASN	A	359	21.253 -11.381-10.599 1.00 39.34
	20	ATOM	409	OD1	ASN	A	359	21.916 -12.422-10.612 1.00 41.27
		ATOM	410	ND2	ASN	Α	359	20.102 -11.255-11.253 1.00 38.58
		ATOM	411	C	ASN	A	359	22.476 -9.436 -7.510 1.00 30.75
				0	ASN	A	359	23.686 -9.629 -7.412 1.00 33.35
	26	MOTA	412		TRP		360	21.872 -8.400 -6.940 1.00 30.07
1	25	MOTA	413	N		A		22.634 -7.451 -6.132 1.00 27.87
10		MOTA	414	CA	TRP	A	360	
111		MOTA	415	CB	TRP	A	360	
113		ATOM	416	CG	TRP	A	360	
1.4		ATOM	417	CD2	TRP	A	360	21.00
34	30	MOTA	418	CE2	TRP	A	360	22.147 -4.543 -2.564 1.00 22.31
(Like		MOTA	419	CE3	TRP	Α	360	20.392 -6.165 -2.972 1.00 20.09
1		ATOM	420	CD1	TRP	A	360	23.212 -4.488 -4.529 1.00 18.99
19		ATOM	421	NE1	TRP	A	360	23.187 -3.974 -3.255 1.00 21.17
		ATOM	422	CZ2	TRP	A	360	21.721 -4.340 -1.243 1.00 20.43
(1) (J	35	ATOM	423	CZ3	TRP	A	360	19.968 -5.965 -1.661 1.00 20.12
1,1,7	33	ATOM	424	CH2	TRP	A	360	20.635 -5.057 -0.812 1.00 18.54
117				C	TRP	A	360	22.892 -8.099 -4.766 1.00 24.88
1		ATOM	425		TRP	A	360	23.978 -7.980 -4.198 1.00 25.00
10		ATOM	426	0			361	21.879 -8.789 -4.252 1.00 24.08
10		MOTA	427	N	ALA	A		21.972 -9.462 -2.958 1.00 26.06
	40	ATOM	428	CA	ALA	A	361	
		ATOM	429	CB	ALA	Α	361	20.070
		ATOM	430	C	ALA	Α	361	
		ATOM	431	0	ALA	A	361	25.015 20.002 2
		ATOM	432	N	LYS	A	362	23.414 -11.144 -3.992 1.00 31.41
	45	ATOM	433	CA	LYS	A	362	24.530 -12.097 -4.047 1.00 33.33
		ATOM	434	CB	LYS	A	362	24.564 -12.824 -5.390 1.00 34.81
		ATOM	435	CG	LYS	A	362	23.319 -13.608 -5.756 1.00 36.27
		ATOM	436	CD	LYS	A	362	23.458 -14.178 -7.167 1.00 38.30
		ATOM	437	CE	LYS	Α	362	22.369 -15.193 -7.472 1.00 40.94
	50		438	NZ	LYS	A	362	22.111 -15.322 -8.937 1.00 42.49
	30	ATOM		C	LYS	A	362	25.854 -11.351 -3.893 1.00 34.17
		MOTA	439			A	362	26.880 -11.977 -3.595 1.00 35.40
		MOTA	440	0	LYS			25.826 -10.059 -4.095 0.50 34.23
		MOTA	441	N	AARG		363	25.020 10.000
		MOTA	442	N	BARG		363	23.020
	55	MOTA	443	CA	AARG		363	27.055
		MOTA	444	CA	BARG		363	27.035 -9.254 -3.987 0.50 32.83
		ATOM	445	CB	AARG	A	363	27.031 -8.153 -5.044 0.50 34.67
		ATOM	446	CB	BARG	A	363	27.031 -8.153 -5.045 0.50 34.20
		ATOM	447	CG	AARG		363	26.933 -8.654 -6.478 0.50 36.32
	60	ATOM	448	CG	BARG		363	26.930 -8.654 -6.480 0.50 35.56
	00	ATOM	449	CD	AARG		363	27.745 -7.775 -7.415 0.50 38.39
			450	CD	BARG		363	27.752 -7.781 -7.414 0.50 37.18
		ATOM	450	CD	DMICO	21	505	=

	5	ATOM	451	NE	AARG	A	363	29.171 -7.793 -7.091 0.50 39.98	
	3		452	NE	BARG	A	363	27.195 -7.725 -8.762 0.50 37.39	
		MOTA			AARG	A	363	30.086 -7.038 -7.692 0.50 40.54	
		ATOM	453	CZ			363	27.905 -7.457 -9.855 0.50 40.02	
		MOTA	454	CZ	BARG	A		29.735 -6.218 -8.675 0.50 38.13	
		MOTA	455	NH1	AARG	A	363		
	10	MOTA	456	NH1	BARG	A	363		
		MOTA	457	NH2	AARG	A	363		
		MOTA	458	NH2	BARG	A	363	2,1011	
		ATOM	459	C	AARG	A	363		
		ATOM	460	C	BARG	A	363		
	15	MOTA	461	0	AARG	A	363	28.223 -7.992 -2.344 0.50 34.18	
		ATOM	462	0	BARG	Α	363	28.223 -7.992 -2.345 0.50 33.43	
		ATOM	463	N	VAL	Α	364	26.215 -8.798 -1.740 1.00 33.12 26.288 -8.240 -0.389 1.00 33.63	
		ATOM	464	CA	VAL	Α	364	20.200	
		ATOM	465	CB	VAL	Α	364		
	20	ATOM	466	CG1	VAL	A	364		
		ATOM	467	CG2	VAL	Α	364	23.7	
		ATOM	468	C	VAL	A	364	27727	
		MOTA	469	0	VAL	A	364		
		ATOM	470	N	PRO	A	365	28.306 -8.626 0.935 1.00 36.08	
(2)	25	ATOM	471	CD	PRO	A	365	28.775 -7.235 0.793 1.00 34.84	
: [3]		ATOM	472	CA	PRO	A	365	29.231 -9.442 1.733 1.00 37.82 30 110 -8.408 2.430 1.00 34.31	
IU		MOTA	473	CB	PRO	A	365	301220	
(13		ATOM	474	CG	PRO	A	365	301221	
Ini.		ATOM	475	C	PRO	A	365	20.330 20.070 20.20	
145	30	MOTA	476	0	PRO	A	365		
anit		ATOM	477	N	GLY	A	366	20.030	
14		ATOM	478	CA	GLY	A	366		
		ATOM	479	C	GLY	A	366	20,772	
13		MOTA	480	0	GLY	A	366	20.000	
1,1	35	ATOM	481	N	PHE	A	367	20.210 22.022	
1,1		MOTA	482	CA	PHE	A	367		
1100		ATOM	483	CB	PHE	A	367		
10		ATOM	484	CG	PHE	A	367		
ıÖ.		MOTA	485	CD1	PHE	A	367		
	40	ATOM	486	CD2	PHE	A	367	22.000	
		MOTA	487	CE1	PHE	A	367		
		ATOM	488	CE2	PHE	A	367	20.535 -12.491 1.373 1.00 27.60 20.118 -13.103 0.196 1.00 26.81	
		ATOM	489	CZ	PHE	A	367	201220 20121	
		ATOM	490	C	PHE	A	367		
	45	ATOM	491	0	PHE	A	367	24.244 -15.398 1.359 1.00 36.55 26.088 -14.694 0.276 1.00 38.28	
		MOTA	492	N	VAL	A	368	26.289 -15.965 -0.420 1.00 42.34	
		MOTA	493	CA	VAL	A	368	27.386 -15.850 -1.504 1.00 41.78	
		ATOM	494	CB	VAL	A	368	26.972 -14.831 -2.550 1.00 44.60	
		MOTA	495	CG1	VAL	A	368	28.707 -15.457 -0.873 1.00 42.23	
	50	MOTA	496	CG2	VAL	A	368	26.664 -17.100 0.533 1.00 43.85	
		ATOM	497	C	VAL	A	368 368	26.469 -18.274 0.216 1.00 44.85	
		ATOM	498	0	VAL	A		27.199 -16.750 1.699 1.00 44.93	
		ATOM	499	N	ASP	A	369	27.579 -17.755 2.688 1.00 44.96	
		MOTA	500	CA	ASP	A	369	28.336 -17.106 3.849 1.00 43.76	
	55	MOTA	501	CB	ASP	A	369	29.608 -16.413 3.404 1.00 43.04	
		MOTA	502	CG	ASP	A	369	30.121 -15.570 4.167 1.00 44.32	
		MOTA	503	OD1	ASP	A	369 369	30.121 -13.370 4.107 1.00 11.32	
		MOTA	504	OD2	ASP	A	369	26.340 -18.465 3.228 1.00 45.89	
	60	MOTA	505	C	ASP ASP	A A	369	26.360 -19.671 3.475 1.00 48.61	
	60	MOTA	506	N	LEU	A	370	25.261 -17.714 3.407 1.00 43.59	
		MOTA	507	CA	LEU	A	370	24.020 -18.279 3.924 1.00 44.24	
		MOTA	508	CA	טפת	~	5,0	150	

5	3 171034	509	CB	LEU	A	370	22.980 -17.173 4.110 1.00 41.42
,	MOTA	510	CG	LEU	A	370	23.404 -16.015 5.014 1.00 41.45
	MOTA	511	CD1	LEU	A	370	22.219 -15.095 5.245 1.00 42.25
	MOTA	512	CD2	LEU	A	370	23.931 -16.552 6.332 1.00 38.35
	MOTA	513	C	LEU	A	370	23.449 -19.360 3.013 1.00 44.03
10	MOTA		0	LEU	A	370	23.773 -19.423 1.829 1.00 43.63
10	ATOM	514	N	THR	A	371	22.593 -20.206 3.575 1.00 44.29
	ATOM	515	CA	THR	A	371	21.968 -21.272 2.806 1.00 44.84
	ATOM	516			A	371	21.293 -22.302 3.730 1.00 45.65
	ATOM	517	CB	THR	A	371	20.262 -21.663 4.495 1.00 46.43
	MOTA	518	OG1	THR			22.314 -22.903 4.677 1.00 46.48
15	MOTA	519	CG2	THR	A	371	20.923 -20.684 1.864 1.00 44.93
	MOTA	520	C	THR	A	371	20.525
	MOTA	521	0	THR	A	371	20.110
	MOTA	522	N	LEU	A	372	20.007 21.110 7.11
	ATOM	523	CA	LEU	A	372	13.000
20	MOTA	524	CB	LEU	A	372	
	ATOM	525	CG	LEU	A	372	10.012
	ATOM	526	CD1	LEU	Α	372	13.000
	ATOM	527	CD2	LEU	Α	372	10.521 20.011
	MOTA	528	C	LEU	А	372	18.307 -20.644 0.512 1.00 44.84
25	MOTA	529	0	LEU	Α	372	17.705 -19.602 0.261 1.00 43.25
153	ATOM	530	N	HIS	Α	373	17.849 -21.558 1.382 1.00 43.14
111	ATOM	531	CA	HIS	A	373	16.599 -21.353 2.100 1.00 42.23
133	MOTA	532	CB	HIS	A	373	16.318 -22.525 3.062 1.00 45.38
- Inde	MOTA	533	CG	HIS	Α	373	15.114 -22.315 3.934 1.00 51.43
14 30	MOTA	534	CD2	HIS	Α	373	13.808 -22.621 3.743 1.00 54.99
1.4	ATOM	535	ND1	HIS	A	373	15.187 -21.716 5.174 1.00 54.26
N	ATOM	536	CE1	HIS	A	373	13.979 -21.663 5.709 1.00 53.77
31	ATOM	537	NE2	HIS	A	373	13.124 -22.206 4.861 1.00 55.27
(*)	MOTA	538	C	HIS	A	373	16.665 -20.047 2.885 1.00 39.78
10 35	ATOM	539	0	HIS	A	373	15.677 -19.324 2.971 1.00 37.71
W	ATOM	540	N	ASP	Α	374	17.839 -19.738 3.440 1.00 36.38
13	ATOM	541	CA	ASP	A	374	18.020 -18.516 4.219 1.00 37.21
Ō	ATOM	542	CB	ASP	A	374	19.287 -18.620 5.073 1.00 38.17
	ATOM	543	CG	ASP	A	374	19.064 -19.425 6.344 1.00 41.47
40	ATOM	544	OD1	ASP	A	374	17.896 -19.543 6.772 1.00 37.09
	ATOM	545	OD2	ASP	A	374	20.052 -19.940 6.912 1.00 44.40
	ATOM	546	C	ASP	А	374	18.083 -17.277 3.326 1.00 37.19
	ATOM	547	ō	ASP	A	374	17.598 -16.208 3.696 1.00 38.13
	ATOM	548	N	GLN	Α	375	18.688 -17.431 2.152 1.00 33.13
45	ATOM	549	CA	GLN	Α	375	18.788 -16.339 1.198 1.00 31.94
	ATOM	550	CB	GLN	A	375	19.634 -16.756 -0.001 1.00 28.81
	ATOM	551	CG	GLN	А	375	21.125 -16.570 0.189 1.00 31.71
	ATOM	552	CD	GLN	А	375	21.920 -17.222 -0.922 1.00 34.49
	ATOM	553	OE1	GLN	A	375	21.478 -17.267 -2.067 1.00 36.09
50	ATOM	554	NE2	GLN	A	375	23.097 -17.736 -0.588 1.00 40.32
30	ATOM	555	C	GLN	A	375	17.379 -16.009 0.730 1.00 31.50
	ATOM	556	0	GLN	A	375	16.990 -14.840 0.653 1.00 27.42
			N	VAL	A	376	16.617 -17.056 0.429 1.00 30.38
	ATOM	557	CA	VAL	A	376	15.242 -16.907 -0.027 1.00 33.50
	MOTA	558		VAL	A	376	14.588 -18.286 -0.286 1.00 30.57
55		559	CB		A	376	13.093 -18.122 -0.516 1.00 33.14
	MOTA	560	CG1	VAL	A	376	15.232 -18.952 -1.485 1.00 30.79
	ATOM	561	CG2	VAL		376	14.393 -16.159 1.002 1.00 33.80
	ATOM	562	C	VAL	A		13.653 -15.237 0.661 1.00 34.89
	MOTA	563	0	VAL	A	376	14.500 -16.568 2.261 1.00 33.35
60		564	N	HIS	A	377	13.730 -15.941 3.329 1.00 32.81
	ATOM	565	CA	HIS	A	377	13.730 -15.941 3.329 1.00 32.01
	MOTA	566	CB	HIS	A	377	13.700 -10.074 4.014 2.00 33.24

	5	ATOM	567	CG	HIS	A	377	13.429	-15.989	5.851	1.00	40.15
		ATOM	568	CD2	HIS	A	377	14.054	-15.495	6.946	1.00	40.86
		ATOM	569	ND1	HIS	A	377	12.090	-15.703	6.012	1.00	43.08
		ATOM	570	CE1	HIS	Α	377	11.913	-15.062	7.154	1.00	42.44
		ATOM	571	NE2	HIS	A	377	13.089	-14.922	7.740	1.00	44.85
	10	ATOM	572	C	HIS	A	377	14.058	-14.454	3.507	1.00	28.63
		ATOM	573	Ö	HIS	A	377	13.158	-13.619	3.613	1.00	29.20
		ATOM	574	N	LEU	A	378	15.343	-14.125	3.544	1.00	24.41
			575	CA	LEU	A	378	15.759	-14.125	3.721	1.00	23.21
		ATOM ATOM	576	CB	LEU	A	378		-12.738	3.743	1.00	20.98
	1.5											
	15	ATOM	577	CG	LEU	A	378	17.960	-13.190	5.016	1.00	24.22
		MOTA	578	CD1	LEU	A	378		-13.041	4.924	1.00	21.07
		ATOM	579	CD2	LEU	Α	378	17.431	-12.446	6.221	1.00	20.24
		MOTA	580	C	LEU	A	378		-11.827	2.630	1.00	24.78
		ATOM	581	0	LEU	Α	378		-10.766	2.922	1.00	22.09
	20	MOTA	582	N	LEU	A	379		-12.242	1.374	1.00	24.13
		MOTA	583	CA	LEU	Α	379	14.812	-11.447	0.262	1.00	25.02
		ATOM	584	CB	LEU	A	379	15.307	-12.025	-1.062	1.00	27.12
		ATOM	585	CG	LEU	A	379	16.724	-11.600	-1.437	1.00	24.39
		ATOM	586	CD1	LEU	A	379	17.299	-12.557	-2.470	1.00	27.58
100	25	ATOM	587	CD2	LEU	A	379	16.679	-10.178	-1.983	1.00	29.05
125		MOTA	588	C	LEU	A	379	13.287	-11.355	0.246	1.00	27.61
112		ATOM	589	0	LEU	A	379	12.726	-10.301	-0.062	1.00	26.16
(1)		ATOM	590	N	GLU	А	380	12.616	-12.454	0.576	1.00	25.65
g _{arts}		ATOM	591	CA	GLU	A	380	11.154	-12.471	0.592	1.00	26.85
143	30	ATOM	592	CB	GLU	Α	380	10.640	-13.882	0.871	1.00	29.38
fud.		ATOM	593	CG	GLU	A	380	10.718	-14.796		1.00	35.58
14		ATOM	594	CD	GLU	A	380	10.228		-0.025	1.00	39.31
81		ATOM	595	OE1	GLU	A	380	10.142	-17.008		1.00	42.89
114.5		ATOM	596	OE2	GLU	A	380	9.927	-16.478	1.153	1.00	39.45
141	35	ATOM	597	C	GLU	A	380		-11.526	1.649	1.00	25.43
Lil.	55	ATOM	598	o	GLU	A	380	9.551	-10.925	1.469	1.00	27.75
75		ATOM	599	N	CYS	A	381	11.324	-11.400	2.753	1.00	25.57
(C)		ATOM	600	CA	CYS	A	381	10.907	-10.530	3.843	1.00	26.46
Ď		ATOM	601	CB	CYS	A	381	11.570	-11.000	5.149	1.00	31.46
ind.	40	ATOM	602	SG	CYS	A	381	11.305	-9.946	6.623	1.00	45.32
	40	ATOM	603	C	CYS	A	381	11.262	-9.059	3.589	1.00	24.77
					CYS	A	381		-8.166	3.975	1.00	25.01
		ATOM	604	O N		A		10.516			1.00	22.23
		ATOM	605		ALA		382	12.377	-8.815	2.903		
	45	ATOM	606	CA	ALA	A	382	12.855	-7.449	2.681	1.00	21.83
	43	ATOM	607	CB	ALA	A	382	14.319	-7.383	3.095	1.00	21.56
		ATOM	608	C	ALA	A	382	12.705	-6.778	1.311	1.00	19.78
		ATOM	609	0	ALA	A	382	12.996	-5.587	1.182	1.00	17.01
		ATOM	610	N	TRP	A	383	12.261	-7.507	0.294	1.00	17.61
	=0	MOTA	611	CA	TRP	A	383	12.164	-6.915		1.00	18.06
	50	MOTA	612	CB	TRP	A	383	11.580	-7.928		1.00	20.28
		MOTA	613	CG	TRP	A	383	10.105	-8.201		1.00	20.50
		MOTA	614	CD2	TRP	A	383	9.049	-7.509		1.00	22.48
		ATOM	615	CE2	TRP	A	383	7.836	~8.138	-2.238	1.00	20.41
		MOTA	616	CE3	TRP	A	383	9.012	-6.420	-3.482	1.00	22.06
	55	MOTA	617	CD1	TRP	A	383	9.506	-9.189		1.00	23.38
		ATOM	618	NE1	TRP	A	383	8.142	-9.159	-1.377	1.00	22.59
		ATOM	619	CZ2	TRP	A	383	6.598	-7.713	-2.724	1.00	21.98
		ATOM	620	CZ3	TRP	Α	383	7.780	-5.998	-3.968	1.00	25.50
		MOTA	621	CH2	TRP	A	383	6.589	-6.647	-3.587	1.00	23.11
	60	ATOM	622	C	TRP	Α	383	11.448	~5.564	-1.170	1.00	19.18
		ATOM	623	0	TRP	A	383	11.972	-4.663	-1.824	1.00	19.27
		ATOM	624	N	LEU	A	384	10.273	-5.396	-0.567	1.00	18.32

	_					_		0 506	-4.118 -0.719	1.00	16.38
	5	ATOM	625	CA	LEU	A	384	9.586			16.79
		ATOM	626	CB	LEU	A	384	8.125		1.00	
		ATOM	627	CG	LEU	A	384	7.211		1.00	18.39
		MOTA	628	CD1	LEU	A	384	7.464		1.00	13.91
		ATOM	629	CD2	LEU	A	384	5.750		1.00	18.38
	10	ATOM	630	C	LEU	A	384	10.324		1.00	18.80
		ATOM	631	0	LEU	Α	384	10.334		1.00	20.90
		ATOM	632	N	GLU	A	385	10.949	-3.404 1.163	1.00	18.61
		ATOM	633	CA	GLU	Α	385	11.718	-2.462 1.970	1.00	19.58
		ATOM	634	CB	GLU	A	385	12.274	-3.154 3.213	1.00	17.43
	15	ATOM	635	CG	GLU	A	385	11.292	-3.237 4.357	1.00	22.92
	13	ATOM	636	CD	GLU	A	385	11.963	-3.676 5.640	1.00	25.83
				OE1	GLU	A	385	12.431	-2.799 6.391	1.00	23.69
		MOTA	637		GLU	A	385	12.027	-4.897 5.889	1.00	27.64
		ATOM	638	OE2			385	12.890	-1.934 1.156	1.00	19.46
		ATOM	639	C	GLU	A		13.206	-0.743 1.196	1.00	15.04
	20	ATOM	640	0	GLU	A	385		-2.842 0.431	1.00	13.32
		ATOM	641	N	ILE	Α	386	13.539		1.00	15.01
		MOTA	642	CA	ILE	Α	386	14.685	-2.484 -0.388		
		ATOM	643	CB	ILE	Α	386	15.475	-3.763 -0.807	1.00	17.43
		ATOM	644	CG2	ILE	Α	386	16.544	-3.424 -1.849	1.00	17.99
173	25	ATOM	645	CG1	ILE	Α	386	16.185	-4.338 0.432	1.00	20.31
0		ATOM	646	CD1	ILE	A	386	16.682	-5.766 0.284	1.00	23.97
ĮŲ.		ATOM	647	C	ILE	A	386	14.273	-1.645 -1.598	1.00	16.10
10		ATOM	648	0	ILE	A	386	14.993	-0.724 -2.004	1.00	17.42
fot.		ATOM	649	N	LEU	A	387	13.112	-1.944 -2.167	1.00	17.61
141	30	ATOM	650	CA	LEU	Α	387	12.620	-1.173 -3.304	1.00	18.20
	50	ATOM	651	CB	LEU	A	387	11.359	-1.814 -3.882	1.00	17.51
lade.		ATOM	652	CG	LEU	A	387	11.519	-3.064 -4.747	1.00	26.37
14		ATOM	653	CD1	LEU	A	387	10.173	-3.406 -5.395	1.00	24.63
H			654	CD2	LEU	A	387	12.589	-2.824 -5.808	1.00	21.58
	35	ATOM	655	CDZ	LEU	A	387	12.283	0.249 -2.838	1.00	17.60
143	33	ATOM		0	LEU	A	387	12.571	1.224 -3.530	1.00	17.15
14		MOTA	656		MET	A	388	11.677	0.357 -1.660	1.00	17.65
190		ATOM	657	N			388	11.286	1.656 -1.121	1.00	18.49
17		ATOM	658	CA	MET	A		10.302	1.460 0.034	1.00	19.65
(2)		ATOM	659	CB	MET	A	388	8.893	1.105 -0.435	1.00	15.12
	40	ATOM	660	CG	MET	A	388		0.769 0.910	1.00	18.73
		ATOM	661	SD	MET	A	388	7.744	0.908 0.048	1.00	18.34
		MOTA	662	CE	MET	A	388	6.163		1.00	22.62
		ATOM	663	C	MET	A	388	12.451	2.553 -0.691		22.49
		ATOM	664	0	MET	Α	388	12.417	3.767 -0.928	1.00	21.45
	45	ATOM	665	N	ILE	A	389	13.482	1.988 -0.064	1.00	
		ATOM	666	CA	ILE	A	389	14.604	2.831 0.331	1.00	18.54
		ATOM	667	CB	ILE	A	389	15.590	2.108 1.299	1.00	19.35
		ATOM	668	CG2	ILE	Α	389	16.362	0.998 0.578	1.00	15.50
		ATOM	669	CG1	ILE	Α	389	16.556	3.142 1.889	1.00	21.95
	50	ATOM	670	CD1	ILE	Α	389	17.373	2.658 3.080	1.00	15.86
		ATOM	671	C	ILE	A	389	15.333	3.322 -0.922	1.00	18.67
		ATOM	672	ō	ILE	А	389	15.813	4.453 -0.970	1.00	19.75
		ATOM	673	N	GLY	A	390	15.410	2.477 -1.943	1.00	20.58
		ATOM	674	CA	GLY	A	390	16.049	2.895 -3.183	1.00	19.33
	==		675	C	GLY	A	390	15.243	4.021 -3.819	1.00	17.48
	55	ATOM			GLY	A	390	15.801	4.994 -4.318	1.00	21.87
		ATOM	676	0			391	13.920	3.888 -3.787	1.00	19.17
		MOTA	677	N	LEU	A		13.920	4.887 -4.343	1.00	21.50
		ATOM	678	CA	LEU	A	391		4.420 -4.194	1.00	18.25
		ATOM	679	CB	LEU	A	391	11.561	5.497 -4.342	1.00	21.98
	60	MOTA	680	CG	LEU	A	391	10.480	6.156 -5.725	1.00	21.39
		MOTA	681	CD1	LEU	A	391	10.579		1.00	17.15
		ATOM	682	CD2	LEU	Α	391	9.115	4.868 -4.148	1.00	11.13

5		500	~	LEU	A	391	13.208	6.216 -3.620	1.00	23.27
3	ATOM	683	С О	LEU	A	391	13.440	7.255 -4.243	1.00	23.60
	MOTA	684				392	13.122	6.170 -2.295	1.00	23.04
	ATOM	685	N	VAL	A	392	13.122	7.357 -1.469	1.00	24.42
	MOTA	686	CA	VAL	A			6.993 0.042	1.00	27.38
	MOTA	687	CB	VAL	Α	392	13.186	8.129 0.897	1.00	30.37
10	MOTA	688	CG1	VAL	A	392	13.733		1.00	23.48
	ATOM	689	CG2	VAL	Α	392	11.739	6.712 0.414		27.55
	ATOM	690	C	VAL	A	392	14.626	8.014 -1.754	1.00	
	ATOM	691	0	VAL	A	392	14.728	9.242 -1.832	1.00	27.50
	ATOM	692	N	TRP	Α	393	15.652	7.186 -1.924	1.00	23.65
15	ATOM	693	CA	TRP	Α	393	16.999	7.670 -2.204	1.00	24.76
	ATOM	694	CB	TRP	Α	393	17.977	6.491 -2.199	1.00	22.86
	ATOM	695	CG	TRP	Α	393	19.287	6.784 -2.857	1.00	25.90
	ATOM	696	CD2	TRP	A	393	20.341	7.605 -2.339	1.00	28.09
	ATOM	697	CE2	TRP	A	393	21.375	7.612 -3.302	1.00	29.94
20	ATOM	698	CE3	TRP	A	393	20.512	8.335 -1.154	1.00	30.20
20	ATOM	699	CD1	TRP	A	393	19.710	6.339 -4.077	1.00	26.55
	ATOM	700	NE1	TRP	A	393	20.963	6.833 -4.351	1.00	30.64
	ATOM	701	CZ2	TRP	Α	393	22.566	8.323 -3.120	1.00	32.43
	ATOM	702	CZ3	TRP	A	393	21.698	9.044 -0.971	1.00	34.58
1 25		702	CH2	TRP	A	393	22.709	9.030 -1.950	1.00	36.54
	ATOM	704	C	TRP	A	393	17.082	8.414 -3.547	1.00	25.02
40	ATOM		0	TRP	A	393	17.767	9.435 -3.650	1.00	20.97
17.1	ATOM	705		ARG	A	394	16.399	7.897 -4.568	1.00	23.06
10	ATOM	706	N		A	394	16.412	8.531 -5.890	1.00	25.97
jeda 20	ATOM	707	CA	ARG			15.776	7.633 -6.965	1.00	24.05
30	ATOM	708	CB	ARG	A	394	16.243	6.195 -7.024	1.00	26.05
Seeds	MOTA	709	CG	ARG	Α	394	15.830	5.551 -8.352	1.00	22.70
144	MOTA	710	CD	ARG	A	394	14.443	5.071 -8.363	1.00	20.71
27	ATOM	711	NE	ARG	A	394	14.053	3.912 -7.841	1.00	21.26
0	ATOM	712	CZ	ARG	A	394	14.053	3.108 -7.267	1.00	20.09
1 35	ATOM	713	NH1	ARG	A	394		3.544 -7.907	1.00	21.26
أرارا	MOTA	714	NH2	ARG	A	394	12.783	9.833 -5.879	1.00	23.40
Frank	MOTA	715	C	ARG	A	394	15.622	10.729 -6.677	1.00	28.61
Ď	ATOM	716	0	ARG	A	394	15.889		1.00	26.65
×159	ATOM	717	N	SER	A	395	14.638	9.924 -4.988		27.46
40	ATOM	718	CA	SER	A	395	13.776	11.104 -4.902	1.00	
	ATOM	719	CB	SER	A	395	12.395	10.696 -4.382	1.00	26.70
	ATOM	720	OG	SER	A	395	11.916	9.530 -5.029	1.00	22.95
	ATOM	721	C	SER	Α	395	14.316	12.240 -4.033	1.00	31.45
	ATOM	722	0	SER	A	395	13.726	13.324 -3.977	1.00	28.11
45	ATOM	723	N	MET	A	396	15.437	11.986 -3.368	1.00	33.83
	ATOM	724	CA	MET	A	396	16.061	12.954 -2.475	1.00	38.83
	ATOM	725	CB	MET	Α	396	17.466	12.483 -2.112	1.00	39.47
	ATOM	726	CG	MET	Α	396	17.585	11.919 -0.715	1.00	41.37
	ATOM	727	SD	MET	A	396	19.192	12.262 0.004	1.00	42.20
50	ATOM	728	CE	MET	A	396	20.263	11.996 -1.404	1.00	42.84
	ATOM	729	C	MET	A	396	16.143	14.376 -3.018	1.00	40.69
	ATOM	730	0	MET	A	396	15.637	15.316 -2.403	1.00	38.85
	ATOM	731	N	GLU	A	397	16.794	14.526 -4.166	1.00	42.19
	ATOM	732	CA	GLU	Α	397	16.971	15.831 -4.790	1.00	44.80
55		733	CB	GLU	A	397	18.184	15.785 -5.729	1.00	46.02
	ATOM	734	CG	GLU	Α	397	17.883	15.189 -7.096	1.00	54.42
	ATOM	735	CD	GLU	A	397	19.117	14.665 -7.810	1.00	59.40
	ATOM	736	OE1	GLU	A	397	19.219	13.430 -7.990	1.00	60.63
	ATOM	737	OE2	GLU	A	397	19.980	15.485 -8.196	1.00	62.71
60		738	C	GLU	A	397	15.735	16.322 -5.554	1.00	42.94
00	ATOM	739	0	GLU	A	397	15.830	17.229 -6.376	1.00	44.68
	ATOM	740	N	HIS	A	398	14.579	15.728 -5.280	1.00	40.82
	AIOM	/-= 0	74	1113		330				

										39.21
5	ATOM	741	CA	HIS	Α	398	13.342		1.00	39.05
	ATOM	742	CB	HIS	A	398	12.924		1.00	
	ATOM	743	CG	HIS	A	398	13.870		1.00	41.57
	ATOM	744	CD2	HIS	Α	398	13.904		1.00	39.28
	ATOM	745	ND1	HIS	Α	398	14.940		1.00	41.85
10		746	CE1	HIS	Α	398	15.592	14.086 -9.220	1.00	40.88
	ATOM	747	NE2	HIS	A	398	14.985	14.969 -9.993	1.00	42.30
	ATOM	748	C	HIS	A	398	12.216	16.332 -4.944	1.00	37.04
	ATOM	749	ō	HIS	A	398	11.282	15.535 -4.864	1.00	36.51
	ATOM	750	N	PRO	A	399	12.283	17.427 -4.171	1.00	39.19
15		751	CD	PRO	A	399	13.328		1.00	35.36
13			CA	PRO	A	399	11.243		1.00	37.10
	ATOM	752			A	399	11.603		1.00	37.86
	MOTA	753	CB	PRO		399	13.050		1.00	35.83
	ATOM	754	CG	PRO	Α		9.828		1.00	37.02
	ATOM	755	C	PRO	A	399			1.00	38.52
20		756	0	PRO	Α	399	9.554		1.00	33.58
	ATOM	757	N	GLY	A	400	8.938			32.12
	ATOM	758	CA	GLY	А	400	7.559		1.00	
	ATOM	759	C	GLY	Α	400	7.230		1.00	32.43
	ATOM	760	0	GLY	A	400	6.063		1.00	33.21
25	ATOM	761	N	LYS	Α	401	8.237		1.00	31.35
AD	MOTA	762	CA	LYS	Α	401	7.972		1.00	30.75
111	ATOM	763	CB	LYS	A	401	8.235		1.00	35.43
(2)	ATOM	764	CG	LYS	Α	401	8.130	15.927 -7.675	1.00	35.15
\$ all	MOTA	765	CD	LYS	Α	401	9.096	16.353 -8.774	1.00	36.88
30		766	CE	LYS	A	401	8.733	17.721 -9.331	1.00	36.71
	ATOM	767	NZ	LYS	A	401	7.295	18.027 -9.116	1.00	34.22
1.6	ATOM	768	C	LYS	A	401	8.768	12.746 -5.677	1.00	30.97
***	ATOM	769	0	LYS	A	401	9.809		1.00	27.60
2)		770	N	LEU	A	402	8.256		1.00	27.28
(m)	MOTA			LEU	A	402	8.889		1.00	29.07
(d) 3:		771	CA	LEU	A	402	7.866		1.00	22.55
l.i.l	MOTA	772	CB			402	7.265		1.00	24.94
71905 Extent	MOTA	773	CG	LEU	A	402	6.126		1.00	19.32
1100	MOTA	774	CD1	LEU	A		8.355	9.416 -3.157	1.00	21.54
107	MOTA	775	CD2	LEU	Α	402			1.00	28.78
4		776	C	LEU	A	402	9.448	9.836 -8.389	1.00	29.98
	ATOM	777	0	LEU	A	402	8.704	9.770 -7.487	1.00	27.57
	MOTA	778	N	LEU	Α	403	10.761		1.00	27.17
	MOTA	779	CA	LEU	Α	403	11.393	9.400 -8.744		26.95
	ATOM	780	CB	LEU	Α	403	12.825	9.937 -8.816	1.00	30.42
4	5 ATOM	781	CG	LEU	A	403	13.401	10.027-10.238	1.00	
	ATOM	782	CD1	LEU	Α	403	14.519	11.046-10.288	1.00	30.76
	MOTA	783	CD2	LEU	A	403	13.915	8.665-10.676	1.00	33.11
	ATOM	784	C	LEU	A	403	11.419	7.891 -8.901	1.00	24.78
	ATOM	785	0	LEU	A	403	12.428	7.257 -8.619	1.00	24.68
5	MOTA 0	786	N	PHE	A	404	10.306	7.319 -9.344	1.00	23.11
-	ATOM	787	CA	PHE	A	404	10.239	5.881 -9.546	1.00	26.93
	ATOM	788	CB	PHE	Α	404	8.826	5.470 -9.946	1.00	27.04
	ATOM	789	CG	PHE	Α	404	7.850	5.513 -8.816	1.00	27.89
	ATOM	790	CD1	PHE	A	404	7.028	6.623 -8.631	1.00	26.20
	_	791	CD2	PHE	A	404	7.750	4.444 -7.925	1.00	23.10
3		792	CE1	PHE	A	404	6.116	6.668 -7.573	1.00	25.29
	ATOM			PHE	A	404	6.845	4.481 -6.870	1.00	21.01
	ATOM	793	CE2			404	6.026	5.595 -6.693	1.00	22.91
	ATOM	794	CZ	PHE	A	404	11.232	5.507-10.637	1.00	26.04
	ATOM	795	C	PHE			11.882	4.464-10.578	1.00	27.27
6	MOTA 06	796	0	PHE	A	404		6.383-11.626	1.00	28.80
	MOTA	797	N	ALA	A	405	11.348	6.195-12.740	1.00	29.21
	MOTA	798	CA	ALA	A	405	12.271	0.195-12.740	1.00	27.21

	5	ATOM	799	CB	ALA	A	405	11.650	5.287-13.806	1.00	26.89
	,	ATOM	800	C	ALA	A	405	12.549	7.578-13.317	1.00	30.23
		ATOM	801	0	ALA	A	405	11.770	8.508-13.109	1.00	27.38
		ATOM	802	N	PRO	A	406	13.672	7.737-14.032	1.00	30.05
				CD	PRO	A	406	14.712	6.745-14.352	1.00	26.31
	10	ATOM	803		PRO	A	406	13.977	9.053-14.604	1.00	32.10
	10	ATOM	804	CA			406	15.232	8.800-15.438	1.00	31.28
		MOTA	805	CB	PRO	A			7.602-14.776	1.00	31.44
		ATOM	806	CG	PRO	A	406	15.865	9.589-15.436	1.00	32.58
		ATOM	807	C	PRO	A	406	12.820			32.58
		MOTA	808	0	PRO	Α	406	12.605	10.796-15.507	1.00	
	15	ATOM	809	N	ASN	Α	407	12.063	8.690-16.053	1.00	32.86
		MOTA	810	CA	ASN	Α	407	10.935	9.119-16.865	1.00	32.78
		ATOM	811	CB	ASN	Α	407	10.950	8.418-18.228	1.00	34.73
		ATOM	812	CG	ASN	A	407	10.884	6.907-18.121	1.00	35.37
		ATOM	813	OD1	ASN	Α	407	11.189	6.317-17.077	1.00	30.24
	20	ATOM	814	ND2	ASN	A	407	10.486	6.268-19.215	1.00	34.08
		ATOM	815	C	ASN	Α	407	9.605	8.901-16.166	1.00	34.90
		ATOM	816	ō	ASN	А	407	8.549	8.897-16.798	1.00	36.09
		ATOM	817	N	LEU	A	408	9.660	8.724-14.851	1.00	33.56
		ATOM	818	CA	LEU	A	408	8.452	8.544-14.061	1.00	35.59
	25		819	CB	LEU	A	408	8.141	7.062-13.851	1.00	33.81
3144	25	ATOM				A	408	6.696	6.823-13.397	1.00	36.44
10		MOTA	820	CG	LEU		408	5.746	7.479-14.390	1.00	34.14
IU		MOTA	821	CD1	LEU	A		6.406	5.334-13.287	1.00	32.96
170		MOTA	822	CD2	LEU	A	408		9.245-12.717	1.00	38.03
1 rate		MOTA	823	C	LEU	A	408	8.607	8.614-11.695	1.00	36.38
200	30	ATOM	824	0	LEU	A	408	8.880			37.87
į.a.		ATOM	825	N	LEU	A	409	8.441	10.563-12.741	1.00	37.95
No.		MOTA	826	CA	LEU	А	409	8.548	11.395-11.553	1.00	
#1		MOTA	827	CB	LEU	A	409	9.373	12.636-11.877	1.00	39.52
(20)		ATOM	828	CG	LEU	A	409	10.023	13.399-10.728	1.00	42.46
1,1,1	35	ATOM	829	CD1	LEU	A	409	11.100	12.547-10.082	1.00	43.24
LA.		ATOM	830	CD2	LEU	A	409	10.614	14.691-11.266	1.00	46.05
100		ATOM	831	C	LEU	Α	409	7.132	11.792-11.163	1.00	37.13
100		ATOM	832	0	LEU	A	409	6.482	12.546-11.882	1.00	35.70
1/2		MOTA	833	N	LEU	Α	410	6.654	11.284-10.030	1.00	35.29
3D	40	ATOM	834	CA	LEU	A	410	5.297	11.576 -9.583	1.00	33.33
		ATOM	835	CB	LEU	Α	410	4.503	10.277 -9.449	1.00	29.37
		ATOM	836	CG	LEU	A	410	4.645	9.238-10.560	1.00	32.75
		ATOM	837	CD1	LEU	A	410	4.026	7.925-10.104	1.00	29.16
		ATOM	838	CD2	LEU	A	410	3.958	9.744-11.819	1.00	30.70
	45	ATOM	839	C	LEU	A	410	5.207	12.332 -8.261	1.00	35.14
	43		840	0	LEU	A	410	6.078	12.214 -7.400	1.00	36.94
		ATOM		N	ASP	A	411	4.141	13.108 -8.105	1.00	34.76
		MOTA	841			A	411	3.933	13.843 -6.873	1.00	35.40
		ATOM	842	CA	ASP		411	3.733	15.341 -7.144	1.00	40.02
		MOTA	843	CB	ASP	A		2.471	15.645 -7.928	1.00	41.32
	50	MOTA	844	CG	ASP	A	411		14.785 -8.001	1.00	45.03
		MOTA	845	OD1	ASP	A	411	1.570			45.01
		MOTA	846	OD2	ASP	A	411	2.383	16.764 -8.474	1.00	
		MOTA	847	C	ASP	Α	411	2.727	13.234 -6.179	1.00	36.10
		ATOM	848	0	ASP	Α	411	2.033	12.395 -6.762	1.00	34.08
	55	ATOM	849	N	ARG	Α	412	2.480	13.647 -4.940	1.00	35.99
		MOTA	850	CA	ARG	A	412	1.375	13.099 -4.169	1.00	39.37
		ATOM	851	CB	ARG	A	412	1.260	13.824 -2.825	1.00	39.75
		ATOM	852	CG	ARG	Α	412	0.562	15.168 -2.870	1.00	40.49
		ATOM	853	CD	ARG	A	412	0.454	15.736 -1.465	1.00	40.65
	60	ATOM	854	NE	ARG	A	412	-0.261	14.826 -0.577	1.00	37.48
	00	ATOM	855	CZ	ARG	A	412	-1.574	14.855 -0.384	1.00	42.84
		ATOM	856	NH1	ARG	A	412	-2.316	15.754 -1.024	1.00	40.82
		ALON	0.50					164			

	5	ATOM	857	NH2	ARG	A	412	-2.150	13.986 0.438	1.00	38.32
	,	ATOM	858	C	ARG	A	412	0.034	13.108 -4.889	1.00	39.80
		ATOM	859	ō	ARG	A	412	-0.775	12.201 -4.706	1.00	39.92
		ATOM	860	N	ASN	A	413	-0.198	14.119 -5.717	1.00	41.64
		ATOM	861	CA	ASN	A	413	-1.458		1.00	43.19
	10	ATOM	862	CB	ASN	A	413	-1.518	15.533 -7.210	1.00	46.44
	10	ATOM	863	CG	ASN	A	413	-1.739	16.718 -6.299	1.00	47.86
		ATOM	864	OD1	ASN	A	413	-2.376	16.594 -5.249	1.00	48.05
		ATOM	865	ND2	ASN	A	413	-1.213		1.00	49.43
		ATOM	866	C	ASN	A	413	-1.673		1.00	41.48
	15	ATOM	867	0	ASN	A	413	-2.792	12.567 -7.546	1.00	40.50
	13		868	N	GLN	A	414	-0.600		1.00	42.82
		ATOM ATOM	869	CA	GLN	A	414	-0.703		1.00	44.73
		ATOM	870	CB	GLN	A	414	0.585		1.00	47.52
		ATOM	871	CG	GLN	A	414	0.572		1.00	50.47
	20	ATOM	872	CD	GLN	A	414	1.914		1.00	53.91
	20	ATOM	873	OE1	GLN	A	414	2.591		1.00	53.68
		ATOM	874	NE2	GLN	A	414	2.309		1.00	56.91
				C	GLN	A	414	-0.970	10.163 -8.141	1.00	43.21
		ATOM	875 876	0	GLN	A	414	-1.491	9.193 -8.682	1.00	42.33
	25	ATOM ATOM	877	N	GLY	A	415	-0.618	10.168 -6.860	1.00	41.97
(1)	23	ATOM	878	CA	GLY	A	415	-0.836	8.992 -6.040	1.00	40.43
(1)		ATOM	879	C	GLY	A	415	-2.306	8.720 -5.804	1.00	40.80
TU			880	0	GLY	A	415	-2.696	7.601 -5.472	1.00	37.83
1D		ATOM	881	N	LYS	A	416	-3.129	9.748 -5.978	1.00	42.16
ast.	30	ATOM	882	CA	LYS	A	416	-4.566	9.613 -5.779	1.00	44.34
	30	ATOM ATOM	883	CB	LYS	A	416	-5.212	10.996 -5.704	1.00	45.65
Link			884	CG	LYS	A	416	-4.761	11.819 -4.510	1.00	47.42
14		ATOM ATOM	885	CD	LYS	A	416	-4.910	13.309 -4.777	1.00	50.97
21		ATOM	886	CE	LYS	A	416	-5.992	13.924 -3.898	1.00	53.25
(3)	35	ATOM	887	NZ	LYS	A	416	-5.416	14.764 -2.809	1.00	56.95
W	33	ATOM	888	C	LYS	A	416	-5.227	8.793 -6.886	1.00	45.33
		ATOM	889	0	LYS	A	416	-6.339	8.299 -6.714	1.00	46.50
100		ATOM	890	N	CYS	A	417	-4.540	8.648 -8.015	1.00	45.18
143		ATOM	891	CA	CYS	A	417	-5.066	7.890 -9.148	1.00	46.25
123	40	ATOM	892	CB	CYS	A	417	-4.062	7.902-10.305	1.00	49.29
	40	ATOM	893	SG	CYS	A	417	-3.916	9.493-11.168	1.00	49.59
		ATOM	894	C	CYS	A	417	-5.373	6.452 -8.752	1.00	47.18
		ATOM	895	0	CYS	A	417	-6.220	5.794 -9.359	1.00	46.50
		ATOM	896	N	VAL	A	418	-4.671	5.968 -7.731	1.00	45.07
	45	ATOM	897	CA	VAL	A	418	-4.866	4.612 -7.232	1.00	42.75
	73	ATOM	898	CB	VAL	A	418	-3.525	3.841 -7.206	1.00	42.45
		ATOM	899	CG1	VAL	A	418	-3.670	2.563 -6.410	1.00	40.22
		ATOM	900	CG2	VAL	A	418	-3.071	3.538 -8.634	1.00	38.03
		ATOM	901	C	VAL	A	418	-5.441	4.714 -5.818	1.00	41.46
	50	ATOM	902	0	VAL	A	418	-4.883	5.400 -4.963	1.00	42.08
	50	ATOM	903	N	GLU	A	419	-6.559	4.036 -5.579	1.00	40.95
		ATOM	904	CA	GLU	A	419	-7.223	4.073 -4.275	1.00	42.51
		ATOM	905	CB	GLU	A	419	-8.536	3.282 -4.333	1.00	44.52
		ATOM	906	CG	GLU	A	419	-9.010	2.751 -2.984	1.00	50.42
	55		907	CD	GLU	A	419	-10.413	2.168 -3.035	1.00	54.38
))	ATOM ATOM	908	OE1	GLU	A	419	-10.582	1.059 -3.590	1.00	54.09
		ATOM	909	OE2	GLU	A	419	-11.347	2.820 -2.516	1.00	57.90
		ATOM	910	C	GLU	A	419	-6.370	3.552 -3.121	1.00	41.11
		ATOM	911	0	GLU	A	419	-5.955	2.393 -3.116	1.00	39.42
	60	ATOM	912	N	GLY	A	420	-6.129	4.419 -2.140	1.00	40.53
	00	ATOM	913	CA	GLY	A	420	-5.346	4.049 -0.973	1.00	37.61
		ATOM	914	C	GLY	A	420	-3.854	4.258 -1.140	1.00	37.01
		AT OU	214	_							

						_		2 222	4.105 -	0 100	1.00	32.59
	5	MOTA	915	0	GLY	A	420	-3.088			1.00	36.21
		ATOM	916	N	MET	Α	421	-3.444	4.623 -			36.02
		MOTA	917	CA	MET	Α	421	-2.035	4.825 -		1.00	
		ATOM	918	CB	MET	A	421	-1.799	4.607 -		1.00	32.84
		MOTA	919	CG	MET	Α	421	-0.351	4.754 -		1.00	35.82
	10	ATOM	920	SD	MET	Α	421	0.806	3.611 -		1.00	35.57
		ATOM	921	CE	MET	Α	421	0.881	2.294 -	-5.005	1.00	32.51
		ATOM	922	C	MET	Α	421	-1.474	6.180	-2.226	1.00	34.93
		ATOM	923	0	MET	A	421	-0.275	6.294 -	-1.985	1.00	35.17
		ATOM	924	N	VAL	A	422	-2.319	7.205 -	-2.118	1.00	33.97
	15		925	CA	VAL	A	422	-1.823	8.520	-1.708	1.00	31.29
	13	ATOM	926	CB	VAL	A	422	-2.927	9.607		1.00	33.14
		MOTA			VAL	A	422	-3.823	9.535		1.00	30.10
		ATOM	927	CG1		A	422	-2.279	10.982		1.00	30.08
		ATOM	928	CG2	VAL			-1.231	8.498		1.00	32.64
		ATOM	929	C	VAL	A	422		9.220	0.002	1.00	28.41
	20	ATOM	930	0	VAL	A	422	-0.274	7.670	0.571	1.00	31.53
		MOTA	931	N	GLU	Α	423	-1.803				35.99
		ATOM	932	CA	GLU	A	423	-1.311	7.558	1.935	1.00	
		ATOM	933	CB	GLU	Α	423	-2.190	6.594	2.737	1.00	40.37
		ATOM	934	CG	GLU	A	423	-3.588	7.129	3.043	1.00	49.41
(2)	25	MOTA	935	CD	GLU	Α	423	-4.438	7.336	1.795	1.00	52.38
10		ATOM	936	OE1	GLU	Α	423	-5.349	8.188	1.835	1.00	56.91
17		ATOM	937	OE2	GLU	A	423	-4.200	6.652	0.776	1.00	54.53
10		ATOM	938	C	GLU	A	423	0.127	7.043	1.886	1.00	34.83
link.		ATOM	939	0	GLU	Α	423	1.007	7.552	2.581	1.00	31.85
	30	MOTA	940	N	ILE	Α	424	0.369	6.038	1.050	1.00	30.17
14.2	50	ATOM	941	CA	ILE	A	424	1.711	5.488	0.929	1.00	28.99
100		ATOM	942	CB	ILE	A	424	1.696	4.195	0.109	1.00	30.96
1		ATOM	943	CG2	ILE	A	424	3.108	3.588	0.068	1.00	27.20
В		ATOM	944	CG1	ILE	A	424	0.671	3.230	0.725	1.00	30.77
1457	35		945	CD1	ILE	A	424	0.810	1.787	0.291	1.00	34.69
1.1	33	ATOM		CDI	ILE	A	424	2.700	6.483	0.312	1.00	28.21
W		ATOM	946	0	ILE	A	424	3.856	6.551	0.735	1.00	28.48
15		ATOM	947				425	2.253		-0.675	1.00	27.68
123		ATOM	948	N	PHE	A	425	3.119		-1.315	1.00	27.30
110		ATOM	949	CA	PHE	A	425	2.381		-2.458	1.00	26.36
	40	MOTA	950	CB	PHE	A		2.538		-3.798	1.00	27.22
		ATOM	951	CG	PHE	A	425			-4.958	1.00	27.36
		ATOM	952	CD1	PHE	Α	425	2.619		-3.905	1.00	27.89
		ATOM	953	CD2	PHE	A	425	2.566			1.00	29.63
		MOTA	954	CE1	PHE	A	425	2.721		-6.207	1.00	27.28
	45	ATOM	955	CE2	PHE	A	425	2.668		-5.149		27.28
		ATOM	956	CZ	PHE	Α	425	2.745		-6.303	1.00	
		MOTA	957	C	PHE	Α	425	3.591		-0.312	1.00	25.66
		MOTA	958	0	PHE	A	425	4.757		-0.328	1.00	26.33
		MOTA	959	N	ASP	Α	426	2.680	9.746	0.552	1.00	27.92
	50	ATOM	960	CA	ASP	A	426	2.984	10.759	1.570	1.00	28.88
		ATOM	961	CB	ASP	Α	426	1.721	11.102	2.369	1.00	32.58
		ATOM	962	CG	ASP	A	426	0.781	12.034	1.613	1.00	37.47
		ATOM	963	OD1	ASP	Α	426	-0.432	12.039	1.925	1.00	37.72
		ATOM	964	OD2	ASP	Α	426	1.253	12.758	0.710	1.00	36.35
	55	ATOM	965	C	ASP	A	426	4.071	10.278	2.532	1.00	26.96
	55	ATOM	966	0	ASP	A	426	4.974	11.030	2.900	1.00	27.20
			967	N	MET	A	427	3.978	9.022	2.947	1.00	25.76
		MOTA	968	CA	MET	A	427	4.981	8.468	3.856	1.00	25.89
		ATOM		CB	MET	A	427	4.567	7.070	4.309	1.00	21.17
	C C	ATOM	969	CB	MET	A	427	3.385	7.072	5.257	1.00	24.38
	60	ATOM	970	SD	MET	A	427	3.153	5.489	6.080	1.00	34.32
		ATOM	971		MET	A	427	2.173	4.637	4.910	1.00	21.03
		ATOM	972	CE	MET	м	44/	2.1/3	4.00/	1.520		

	5	ATOM	973	C	MET	A	427	6.321	8.410	3.128	1.00	22.29
	5	ATOM	974	0	MET	A	427	7.363	8.760	3.689	1.00	22.19
		ATOM	975	N	LEU	A	428	6.285	7.985	1.868	1.00	21.75
		ATOM	976	CA	LEU	A	428	7.506	7.892	1.075	1.00	22.91
			977	CB	LEU	A	428	7.202	7.252		1.00	18.47
	10	ATOM		CG	LEU	A	428	6.910	5.747		1.00	19.24
	10	ATOM	978				428	6.278	5.222		1.00	16.82
		MOTA	979	CD1	LEU	A			5.010	0.131	1.00	16.23
		MOTA	980	CD2	LEU	A	428	8.204		0.902	1.00	23.98
		ATOM	981	C	LEU	Α	428	8.148	9.269		1.00	23.06
		ATOM	982	0	LEU	A	428	9.366	9.416	1.034		23.00
	15	ATOM	983	N	LEU	Α	429	7.328	10.281	0.628	1.00	
		ATOM	984	CA	LEU	A	429	7.837	11.642	0.462	1.00	26.29
		ATOM	985	CB	LEU	A	429	6.714	12.571		1.00	27.47
		ATOM	986	CG	LEU	A	429	6.331	12.411		1.00	30.78
		ATOM	987	CD1	LEU	A	429	5.022	13.139		1.00	34.75
	20	ATOM	988	CD2	LEU	Α	429	7.449	12.952	-2.350	1.00	31.96
		ATOM	989	C	LEU	A	429	8.425	12.166	1.776	1.00	25.83
		ATOM	990	0	LEU	A	429	9.482	12.808	1.793	1.00	26.42
		ATOM	991	N	ALA	A	430	7,734	11.890	2.877	1.00	26.45
		ATOM	992	CA	ALA	A	430	8.201	12.333	4.185	1.00	26.11
ine	25		993	CB	ALA	A	430	7.214	11.909	5.265	1.00	23.13
10.0	25	ATOM			ALA	A	430	9.577	11.742	4.462	1.00	25.01
:22		MOTA	994	C				10.455	12.409	5.005	1.00	24.31
10		MOTA	995	0	ALA	A	430	9.767	10.486	4.074	1.00	25.25
		ATOM	996	N	THR	A	431	11.046	9.825	4.294	1.00	22.78
100		MOTA	997	CA	THR	A	431		8.323	3.962	1.00	21.36
1.43	30	MOTA	998	CB	THR	A	431	10.973			1.00	20.27
1.4		ATOM	999	OG1	THR	A	431	9.924	7.727	4.727		19.99
153		ATOM	1000	CG2	THR	A	431	12.291	7.633	4.299	1.00	
71		ATOM	1001	C	THR	A	431	12.103	10.477	3.429	1.00	23.73
\$14G		MOTA	1002	0	THR	A	431	13.234	10.667	3.868	1.00	19.60
1,0	35	ATOM	1003	N	SER	A	432	11.736	10.819	2.197	1.00	24.32
LJ		ATOM	1004	CA	SER	A	432	12.676	11.479	1.301	1.00	26.96
1724		ATOM	1005	CB	SER	A	432	12.067	11.650		1.00	28.70
10		ATOM	1006	OG	SER	A	432	13.084	11.930	-1.039	1.00	33.42
		ATOM	1007	C	SER	A	432	13.033	12.850	1.876	1.00	27.92
10	40	ATOM	1008	ō	SER	A	432	14.176	13.294	1.779	1.00	30.78
		ATOM	1009		SER	Α	433	12.045	13.521	2.459	1.00	28.96
		ATOM	1010	CA	SER	A	433	12.269	14.824	3.076	1.00	34.21
		ATOM	1011		SER	A	433	10.957	15.387	3.623	1.00	35.07
			1011		SER	A	433	10.175	15.961	2.591	1.00	42.38
	45	ATOM			SER	A	433	13.263	14.644	4.223	1.00	33.43
	43	ATOM	1013		SER	A	433	14.152	15.473	4.429	1.00	31.94
		ATOM	1014			A	434	13.105	13.545	4.959	1.00	31.32
		MOTA	1015		ARG			13.980	13.236	6.086	1.00	29.78
		MOTA	1016		ARG	A	434		11.994	6.819	1.00	29.84
		MOTA	1017		ARG	A	434	13.468	11.541	7.983	1.00	32.17
	50	MOTA	1018		ARG	A	434	14.331			1.00	37.00
		ATOM	1019		ARG	A	434	14.626	12.672	8.958		39.44
		ATOM	1020	NE	ARG	A	434	15.321		10.140	1.00	
		ATOM	1021	CZ	ARG	A	434	15.935		11.034	1.00	44.06
		ATOM	1022	NH1	ARG	A	434	15.949		10.885	1.00	45.52
	55	ATOM	1023	NH2	ARG	A	434	16.528		12.084	1.00	45.01
		ATOM	1024		ARG	Α	434	15.413	13.014	5.605	1.00	29.24
		ATOM	1025		ARG	A	434	16.352	13.563	6.173	1.00	29.72
		ATOM	1026		PHE	A	435	15.577	12.206	4.561	1.00	28.95
		ATOM	1027		PHE	A	435	16.901	11.935	4.000	1.00	30.59
	60	ATOM	1028		PHE	A	435	16.777	11.045	2.758	1.00	32.03
	00	ATOM	1029		PHE	A	435	16.795	9.563	3.051	1.00	31.88
		ATOM	1030		PHE	A	435	16.758	9.084		1.00	35.60
		ATOM	1030					167				
								167				

	5	ATOM	1031	CD2	PHE	A	435	16.847	8.643	2.009	1.00	35.89
	,	ATOM	1032	CE1	PHE	A	435	16.771	7.709	4.622	1.00	35.36
		ATOM	1032	CE2	PHE	A	435	16.860	7.271	2.262	1.00	32.71
		ATOM	1033	CZ	PHE	A	435	16.821	6.807	3.570	1.00	33.24
				C	PHE	A	435	17.576	13.253	3.607	1.00	32.73
	10	ATOM	1035		PHE	A	435	18.763	13.464	3.871	1.00	31.16
	10	ATOM	1036	0			436	16.812	14.137	2.975	1.00	33.37
		MOTA	1037	N	ARG	A				2.549	1.00	39.13
		MOTA	1038	CA	ARG	A	436	17.341	15.429	1.756	1.00	40.42
		MOTA	1039	CB	ARG	Α	436	16.282	16.206			43.09
		MOTA	1040	CG	ARG	A	436	16.846	17.317	0.877	1.00	
	15	MOTA	1041	CD	ARG	A	436	15.750	17.960	0.040	1.00	44.53
		ATOM	1042	NE	ARG	Α	436	14.826	16.955		1.00	48.34
		ATOM	1043	CZ	ARG	Α	436	13.530	16.913		1.00	48.81
		ATOM	1044	NH1	ARG	A	436	12.997	17.823	0.619	1.00	47.80
		ATOM	1045	NH2	ARG	Α	436	12.769	15.950	-0.687	1.00	49.53
	20	ATOM	1046	C	ARG	A	436	17.792	16.250	3.753	1.00	38.10
		ATOM	1047	0	ARG	A	436	18.896	16.789	3.764	1.00	41.00
		ATOM	1048	N	MET	A	437	16.936	16.334	4.766	1.00	39.47
		ATOM	1049	CA	MET	A	437	17.257	17.087	5.975	1.00	38.20
		ATOM	1050	CB	MET	A	437	16.102	16.998	6.965	1.00	39.79
-	25	ATOM	1051	C	MET	A	437	18.550	16.594	6.626	1.00	41.15
1,73	23			0	MET	A	437	19.303	17.378	7.201	1.00	40.20
100		MOTA	1052		MET	A	438	18.804	15.285	6.538	1.00	39.65
111		MOTA	1053	N			438	20.011	14.693	7.117	1.00	39.70
(1)		MOTA	1054	CA	MET	A		19.787	13.221	7.463	1.00	39.90
100		ATOM	1055	CB	MET	A	438		12.938	8.460	1.00	41.94
14.	30	MOTA	1056	CG	MET	Α	438	18.694		8.880	1.00	43.12
1.de		MOTA	1057	SD	MET	A	438	18.747	11.188		1.00	43.12
100		MOTA	1058	CE	MET	A	438	20.374	11.064	9.619		38.03
#		ATOM	1059	C	MET	A	438	21.176	14.756	6.142	1.00	
		ATOM	1060	0	MET	A	438	22.321	14.503	6.522	1.00	38.39
	35	ATOM	1061	N	ASN	A	439	20.886	15.070	4.895	1.00	37.64
1:1		MOTA	1062	CA	ASN	Α	439	21.924	15.118	3.895	1.00	35.68
u		ATOM	1063	CB	ASN	A	439	23.019	16.125	4.243	1.00	40.98
1642		ATOM	1064	CG	ASN	A	439	23.933	16.407	3.090	1.00	45.09
ND		ATOM	1065	OD1	ASN	A	439	23.528	16.295	1.934	1.00	47.16
1111	40	ATOM	1066	ND2	ASN	A	439	25.197	16.733	3.372	1.00	46.87
		ATOM	1067	C	ASN	A	439	22.552	13.732	3.739	1.00	31.06
		ATOM	1068	0	ASN	Α	439	23.764	13.581	3.649	1.00	29.54
		ATOM	1069		LEU	A	440	21.692	12.698	3.704	1.00	31.47
		ATOM	1070		LEU	A	440	22.161	11.326	3.579	1.00	31.63
	45	ATOM	1071		LEU	A	440	20.991	10.344	3.380	1.00	33.05
	45	ATOM	1071		LEU	A	440	21.451	8.886	3.209	1.00	37.07
			1072		LEU	A	440	21.957	8.353	4.546	1.00	36.18
		MOTA			LEU	A	440	20.318	8.032	2.682	1.00	32.33
		ATOM	1074				440	23.146	11.161	2.435	1.00	32.10
		MOTA	1075		LEU	A	440	22.925	11.671	1.333	1.00	32.76
	50	MOTA	1076		LEU	A		24.225	10.450	2.702	1.00	32.54
		ATOM	1077		GLN	A	441			1.699	1.00	31.97
		MOTA	1078		GLN	A	441	25.255	10.220		1.00	31.75
		MOTA	1079		GLN	Α	441	26.632	10.320	2.345	1.00	35.56
		MOTA	1080		GLN	A	441	26.896	11.669	2.979		
	55	MOTA	1081	CD	GLN	A	441	27.040	12.748	1.939	1.00	34.97
		ATOM	1082	OE1	GLN	Α	441	27.985	12.782	1.167	1.00	35.51
		MOTA	1083	NE2	GLN	Α	441	26.053	13.659	1.899	1.00	35.41
		MOTA	1084		GLN	A	441	25.100	8.860	1.038	1.00	34.08
		ATOM	1085		GLN	A	441	24.540	7.931	1.625	1.00	30.73
	60	ATOM	1086		GLY	A	442	25.608		-0.187	1.00	32.78
		ATOM	1087		GLY	A	442	25.528	7.503	-0.921	1.00	32.91
		ATOM	1088		GLY	А	442	26.181	6.350	-0.184	1.00	31.87
		111 011		-				168				

	5	ATOM	1089	0	GLY	Α	442	25.642	5.245	-0.154	1.00	33.18
	3			N	GLU	A	443	27.340	6.603	0.416	1.00	30.60
		ATOM	1090			A	443	28.057	5.567	1.150	1.00	30.85
		MOTA	1091	CA	GLU			29.376	6.111	1.704	1.00	32.74
		ATOM	1092	CB	GLU	A	443		6.378	0.646	1.00	36.30
		ATOM	1093	CG	GLU	A	443	30.425			1.00	40.92
	10	ATOM	1094	CD	GLU	Α	443	30.310	7.770	0.066		
		ATOM	1095	OE1	GLU	A	443	29.677	8.630	0.716	1.00	42.27
		ATOM	1096	OE2	GLU	Α	443	30.853		-1.038	1.00	46.82
		ATOM	1097	C	GLU	Α	443	27.206	5.048	2.299	1.00	30.43
		MOTA	1098	0	GLU	A	443	27.211	3.854	2.595	1.00	28.11
	15	ATOM	1099	N	GLU	Α	444	26.482	5.955	2.948	1.00	30.26
		ATOM	1100	CA	GLU	Α	444	25.619	5.589	4.067	1.00	28.18
		ATOM	1101	CB	GLU	Α	444	25.147	6.843	4.797	1.00	26.32
		ATOM	1102	CG	GLU	Α	444	26.250	7.633	5.463	1.00	29.27
		MOTA	1103	CD	GLU	A	444	25.748	8.944	6.023	1.00	29.62
	20	ATOM	1104	OE1	GLU	A	444	25.006	9.652	5.304	1.00	32.00
	20	ATOM	1105	OE2	GLU	A	444	26.088	9.268	7.182	1.00	29.02
			1105	C	GLU	A	444	24.403	4.813	3.572	1.00	26.93
		ATOM		0	GLU	A	444	23.970	3.841	4.191	1.00	24.78
		ATOM	1107		PHE	A	445	23.861	5.256	2.443	1.00	27.79
	25	MOTA	1108	N				22.688	4.633	1.853	1.00	24.50
1)	25	ATOM	1109	CA	PHE	A	445	22.254	5.416	0.610	1.00	25.40
165		ATOM	1110	CB	PHE	Α	445			-0.316	1.00	23.74
1013		ATOM	1111	CG	PHE	Α	445	21.372		-0.004	1.00	23.00
00		MOTA	1112	CD1	PHE	A	445	20.034			1.00	22.37
100		MOTA	1113	CD2	PHE	A	445	21.885		-1.489		22.57
1.1	30	ATOM	1114	CE1	PHE	Α	445	19.215		-0.855	1.00	
i ah		ATOM	1115	CE2	PHE	A	445	21.079		-2.342	1.00	21.69
14		ATOM	1116	CZ	PHE	Α	445	19.741		-2.023	1.00	22.25
16		MOTA	1117	C	PHE	Α	445	22.913	3.169	1.489	1.00	22.81
120g		MOTA	1118	0	PHE	A	445	22.083	2.316	1.796	1.00	22.92
1.0	35	ATOM	1119	N	VAL	Α	446	24.019	2.868	0.822	1.00	22.46
F.L.		ATOM	1120	CA	VAL	Α	446	24.278	1.481	0.447	1.00	22.26
died Trad		ATOM	1121	CB	VAL	Α	446	25.522		-0.465	1.00	22.87
10		ATOM	1122	CG1	VAL	A	446	25.251		-1.799	1.00	22.57
		ATOM	1123	CG2	VAL	Α	446	26.735	1.968	0.217	1.00	22.38
:E	40	ATOM	1124	C	VAL	A	446	24.467	0.614	1.694	1.00	23.68
		ATOM	1125	0	VAL	Α	446	24.177	-0.586	1.680	1.00	22.91
		ATOM	1126		CYS	A	447	24.962	1.223	2.770	1.00	22.02
		ATOM	1127		CYS	Α	447	25.155	0.503	4.025	1.00	24.17
		ATOM	1128		CYS	A	447	25.953	1.359	5.011	1.00	23.95
	45	ATOM	1129		CYS	A	447	27.738	1.324	4.731	1.00	28.57
	-13	ATOM	1130		CYS	A	447	23.781	0.178	4.618	1.00	21.14
		ATOM	1131		CYS	A	447	23.512	-0.960	5.002	1.00	19.37
		ATOM	1132		LEU	A	448	22.915	1.186	4.680	1.00	19.28
			1132		LEU	A	448	21.568	1.002	5.219	1.00	21.31
	50	MOTA	1134		LEU	A	448	20.803	2.324	5.207	1.00	21.90
	30	ATOM			LEU	A	448	21.142	3.337	6.303	1.00	26.61
		ATOM	1135			A	448	20.328	4.594	6.072	1.00	27.74
		MOTA	1136		LEU		448	20.320	2.760	7.672	1.00	24.03
		ATOM	1137		LEU	A		20.827	-0.038	4.442	1.00	21.72
		MOTA	1138		LEU	A	448		-0.803	5.030	1.00	20.87
	55	MOTA	1139		LEU	A	448	20.006			1.00	21.42
		MOTA	1140		LYS	Α	449	20.929	-0.055	3.119	1.00	20.98
		ATOM	1141		LYS	A	449	20.205	-0.997	2.269		
		ATOM	1142		LYS	Α	449	20.440	-0.659	0.788	1.00	21.55
		MOTA	1143		LYS	A	449	19.438		-0.173	1.00	24.82
	60	MOTA	1144		LYS	A	449	19.456		-1.542	1.00	23.33
		MOTA	1145	CE	LYS	A	449	20.816		-2.229	1.00	23.58
		MOTA	1146	NZ	LYS	A	449	20.741	-0.482	-3.698	1.00	28.77
								1.00				

	5	MOTA	1147	C	LYS	Α	449	20.629	-2.436	2.548	1.00	20.33
		ATOM	1148	ō	LYS	A	449	19.800		2.552	1.00	20.57
			1149	N	SER	A	450	21.924		2.777	1.00	19.25
		ATOM			SER	A	450	22.451		3.074	1.00	21.84
		MOTA	1150	CA						3.041	1.00	20.59
		ATOM	1151	CB	SER	A	450	23.982				29.78
	10	ATOM	1152	OG	SER	A	450	24.460		1.702	1.00	
		ATOM	1153	C	SER	A	450	21.975		4.454	1.00	21.58
		MOTA	1154	0	SER	A	450	21.728		4.682	1.00	20.06
		ATOM	1155	N	ILE	Α	451	21.853		5.369	1.00	22.20
		MOTA	1156	CA	ILE	A	451	21.385		6.726	1.00	22.82
	15	MOTA	1157	CB	ILE	Α	451	21.452	-2.476	7.616	1.00	19.62
		ATOM	1158	CG2	ILE	A	451	20.593	-2.658	8.886	1.00	21.11
		ATOM	1159	CG1	ILE	A	451	22.909	-2.210	7.999	1.00	22.20
		ATOM	1160	CD1	ILE	A	451	23.115	-0.960	8.850	1.00	24.48
		ATOM	1161	C	ILE	A	451	19.952		6.662	1.00	21.82
	20	ATOM	1162	0	ILE	A	451	19.575		7.369	1.00	21.72
	20	ATOM	1163	N	ILE	A	452	19.152		5.795	1.00	20.18
				CA	ILE	A	452	17.763		5.649	1.00	18.13
		ATOM	1164					17.703		4.627	1.00	19.72
		ATOM	1165	CB	ILE	A	452			4.169	1.00	18.99
		ATOM	1166	CG2	ILE	A	452	15.720				18.33
100	25	ATOM	1167	CG1	ILE	A	452	16.725		5.282	1.00	
113		ATOM	1168	CD1	ILE	A	452	16.284		4.306	1.00	23.25
113		MOTA	1169	C	ILE	A	452	17.725		5.191	1.00	19.50
127		ATOM	1170	0	ILE	Α	452	16.980		5.737	1.00	17.60
j.d.		ATOM	1171	N	LEU	Α	453	18.555		4.209	1.00	19.23
4	30	ATOM	1172	CA	LEU	A	453	18.589	-7.205	3.679	1.00	21.60
1.4		ATOM	1173	CB	LEU	A	453	19.624	-7.316	2.554	1.00	21.50
14		ATOM	1174	CG	LEU	Α	453	19.835	-8.729	1.989	1.00	25.06
		ATOM	1175	CD1	LEU	A	453	18.550	-9.250	1.364	1.00	25.27
\$1 com-		ATOM	1176	CD2	LEU	Α	453	20.948	-8.694	0.953	1.00	24.73
	35	ATOM	1177	C	LEU	Α	453	18.906	-8.245	4.746	1.00	19.41
1,1,2	33	ATOM	1178	0	LEU	A	453	18.198		4.891	1.00	20.75
14		ATOM	1179	N	LEU	A	454	19.966		5.499	1.00	21.35
13		ATOM	1180	CA	LEU	A	454	20.410		6.530	1.00	23.67
100		ATOM	1181	CB	LEU	A	454	21.870		6.878	1.00	20.69
1 153	40				LEU	A	454	22.816		5.673	1.00	24.92
	40	ATOM	1182	CG		A	454	24.222		6.132	1.00	24.27
		ATOM	1183	CD1	LEU			22.785		4.952	1.00	22.84
		MOTA	1184	CD2	LEU	A	454			7.807	1.00	26.06
		MOTA	1185	C	LEU	A	454	19.572			1.00	27.44
		MOTA	1186	0	LEU	A	454	19.413		8.438		
	45	MOTA	1187	N	ASN	A	455	19.01		8.167	1.00	25.01
		MOTA	1188	CA	ASN	A	455	18.240		9.400	1.00	26.10
		ATOM	1189	CB	ASN	Α	455	18.439		10.002	1.00	22.67
		ATOM	1190	CG	ASN	Α	455	17.62		11.264	1.00	26.67
		ATOM	1191	OD1	ASN	Α	455	17.899	9 -6.751	12.270	1.00	25.16
	50	ATOM	1192	ND2	ASN	A	455	16.61	5 -5.246	11.212	1.00	20.73
	-	ATOM	1193	C	ASN	Α	455	16.739	-7.957	9.418	1.00	25.78
		ATOM	1194	0	ASN	A	455	16.230	-8.516	10.380	1.00	29.22
		ATOM	1195	N	SER	A	456	16.02		8.381	1.00	28.51
		ATOM	1196	CA	SER	A	456	14.57			1.00	32.52
	55		1197	CB	SER	A	456	14.01		7.033	1.00	35.98
	33	ATOM		OG	SER	A	456	14.26			1.00	30.88
		ATOM	1198					14.20		8.711	1.00	33.00
		MOTA	1199		SER	A	456				1.00	33.00
		MOTA	1200	0	SER	A	456	13.11			1.00	28.40
		ATOM	1201		GLY	A	457	14.59				36.28
	60	ATOM	1202		GLY	A	457	14.11			1.00	
		MOTA	1203	C	GLY	A	457	15.05			1.00	40.41
		MOTA	1204	0	GLY	A	457	14.83	1 -13.486	9.456	1.00	38.20
								170				

	5	ATOM	1205	N	VAL	A	458	16.095 -11.657 9.820 1.00 44.13
		ATOM	1206	CA	VAL	A	458	17.079 -12.356 10.647 1.00 51.09
		ATOM	1207	CB	VAL	A	458	18.214 -11.399 11.095 1.00 51.06
		ATOM	1208	CG1	VAL	A	458	17.688 -10.390 12.104 1.00 51.75
		ATOM	1209	CG2	VAL	A	458	19.365 -12.199 11.692 1.00 50.65
	10	ATOM	1210	C	VAL	A	458	16.513 -13.060 11.885 1.00 57.26
		ATOM	1211	0	VAL	A	458	17.085 -14.045 12.356 1.00 58.77
		ATOM	1212	N	TYR	A	459	15.401 -12.560 12.416 1.00 62.31
		ATOM	1213	CA	TYR	A	459	14.793 -13.177 13.592 1.00 68.49
		ATOM	1214	CB	TYR	A	459	14.293 -12.100 14.560 1.00 70.46
	15	ATOM	1215	CG	TYR	Α	459	15.396 -11.196 15.069 1.00 71.73
		ATOM	1216	CD1	TYR	A	459	15.127 -9.888 15.462 1.00 71.93
		ATOM	1217	CE1	TYR	Α	459	16.147 -9.045 15.898 1.00 72.60
		ATOM	1218	CD2	TYR	A	459	16.716 -11.644 15.128 1.00 72.77
		ATOM	1219	CE2	TYR	Α	459	17.741 -10.812 15.560 1.00 73.55
	20	ATOM	1220	CZ	TYR	A	459	17.450 -9.514 15.941 1.00 72.93
		ATOM	1221	OH	TYR	A	459	18.467 -8.687 16.351 1.00 74.56
		ATOM	1222	C	TYR	A	459	13.649 -14.097 13.187 1.00 71.86
		ATOM	1223	0	TYR	A	459	13.380 -15.099 13.852 1.00 73.11
		ATOM	1224	N	THR	A	460	12.981 -13.756 12.090 1.00 74.84
(14)	25	ATOM	1225	CA	THR	A	460	11.881 -14.567 11.589 1.00 77.66
100		ATOM	1226	CB	THR	A	460	11.246 -13.900 10.373 1.00 76.69
1112		ATOM	1227	C	THR	A	460	12.436 -15.938 11.212 1.00 80.26
00		ATOM	1228	0	THR	A	460	11.684 -16.866 10.912 1.00 80.82
ins.		ATOM	1229	N	PHE	A	461	13.762 -16.051 11.231 1.00 82.69
14	30	ATOM	1230	CA	PHE	A	461	14.440 -17.299 10.905 1.00 85.63
lui.		MOTA	1231	CB	PHE	A	461	15.920 -17.034 10.630 1.00 85.47
1		ATOM	1232	C	PHE	A	461	14.284 -18.288 12.059 1.00 87.52
11		ATOM	1233	0	PHE	A	461	14.493 -17.940 13.224 1.00 86.53
5		ATOM	1234	N	LEU	A	462	13.914 -19.520 11.724 1.00 89.49
1,00	35	MOTA	1235	CA	LEU	A	462	13.711 -20.568 12.718 1.00 91.34
14		MOTA	1236	CB	LEU	A	462	12.961 -21.741 12.087 1.00 91.23
1,1,2		ATOM	1237	C	LEU	A	462	15.016 -21.060 13.340 1.00 92.05
1/2		ATOM	1238	0	LEU	A	462	16.042 -21.165 12.664 1.00 91.91
		ATOM	1239	N	SER	Α	463	14.966 -21.357 14.635 1.00 92.53
4D	40	ATOM	1240	CA	SER	A	463	16.131 -21.855 15.358 1.00 92.96
		ATOM	1241	CB	SER	A	463	16.033 -21.483 16.833 1.00 91.67
		ATOM	1242	C	SER	A	463	16.189 -23.371 15.200 1.00 93.39
		ATOM	1243	0	SER	A	463	15.156 -24.034 15.102 1.00 93.44
		ATOM	1244	N	SER	Α	464	17.399 -23.917 15.167 1.00 93.82
	45	ATOM	1245	CA	SER	A	464	17.577 -25.355 15.015 1.00 93.85
		ATOM	1246	CB	SER	A	464	17.284 -25.769 13.577 1.00 93.74
		ATOM	1247	C	SER	A	464	18.997 -25.743 15.396 1.00 93.96
		ATOM	1248	0	SER	Α	464	19.815 -26.074 14.535 1.00 93.65
		ATOM	1249	N	THR	A	465	19.279 -25.699 16.694 1.00 93.91
	50	ATOM	1250	CA	THR	A	465	20.600 -26.036 17.212 1.00 93.79
		ATOM	1251	CB	THR	Α	465	20.952 -27.483 16.863 1.00 93.38
		ATOM	1252	C	THR	A	465	21.640 -25.085 16.634 1.00 93.27
		ATOM	1253	0	THR	Α	465	21.302 -24.017 16.121 1.00 93.03
		ATOM	1254	N	LEU	A	466	22.907 -25.479 16.723 1.00 93.26
	55	ATOM	1255	CA	LEU	A	466	23.999 -24.665 16.207 1.00 92.34
		ATOM	1256	CB	LEU	A	466	25.335 -25.338 16.498 1.00 91.59
		MOTA	1257	C	LEU	Α	466	23.829 -24.461 14.706 1.00 92.18
		ATOM	1258	0	LEU	Α	466	24.411 -23.545 14.125 1.00 92.67
		ATOM	1259	N	LYS	A	467	23.028 -25.323 14.086 1.00 91.28
	60	MOTA	1260		LYS	A	467	22.772 -25.238 12.653 1.00 90.02
		MOTA	1261	. CB	LYS	A	467	21.740 -26.287 12.240 1.00 89.93
		ATOM	1262	C C	LYS	A	467	22.269 -23.841 12.308 1.00 88.35
								171

	5	ATOM	1263	0	LYS	А	467	23.032 -22.990 11.849 1.00 88.50	
	,	ATOM	1264	N	SER	A	468	20.981 -23.610 12.536 1.00 86.02	
				CA	SER	A	468	20.384 -22.315 12.252 1.00 84.10	
		ATOM	1265	CB	SER	A	468	18.901 -22.333 12.620 1.00 84.08	
		ATOM	1266					18.229 -23.378 11.937 1.00 83.03	
		ATOM	1267	OG	SER	A	468	20122	
	10	ATOM	1268	C	SER	A	468		
		ATOM	1269	0	SER	A	468		
		MOTA	1270	N	LEU	Α	469	21.558 -21.579 14.242 1.00 82.04	
		ATOM	1271	CA	LEU	A	469	22.276 -20.640 15.098 1.00 80.28	
		ATOM	1272	CB	LEU	Α	469	22.595 -21.294 16.436 1.00 79.81	
	15	ATOM	1273	C	LEU	A	469	23.564 -20.174 14.419 1.00 79.18	
		ATOM	1274	0	LEU	A	469	24.111 -19.122 14.756 1.00 78.61	
		ATOM	1275	N	GLU	A	470	24.044 -20.969 13.466 1.00 76.69	
		ATOM	1276	CA	GLU	A	470	25.256 -20.638 12.726 1.00 74.84	
		ATOM	1277	CB	GLU	A	470	25.803 -21.880 12.032 1.00 74.12	
	20	ATOM	1278	C	GLU	A	470	24.920 -19.565 11.697 1.00 73.77	
		ATOM	1279	0	GLU	A	470	25.617 -18.556 11.581 1.00 72.94	
		ATOM	1280	N	GLU	A	471	23.842 -19.792 10.953 1.00 72.08	
		ATOM	1281	CA	GLU	A	471	23.396 -18.842 9.945 1.00 70.05	
		ATOM	1282	CB	GLU	A	471	22.461 -19.526 8.944 1.00 71.52	
13	25	ATOM	1283	CG	GLU	А	471	23.150 -19.976 7.668 1.00 72.90	
		ATOM	1284	CD	GLU	А	471	24.512 -20.586 7.932 1.00 74.01	
10		ATOM	1285	OE1	GLU	А	471	25.469 -20.258 7.198 1.00 74.22	
IU		ATOM	1286	OE2	GLU	A	471	24.626 -21.395 8.878 1.00 75.18	
111		ATOM	1287	C	GLU	A	471	22.667 -17.692 10.630 1.00 67.33	
just-	30	ATOM	1288	ō	GLU	A	471	21.685 -17.165 10.107 1.00 67.77	
114	30	ATOM	1289	N	LYS	A	472	23.152 -17.319 11.811 1.00 62.63	
gard.		ATOM	1290	CA	LYS	A	472	22.564 -16.229 12.578 1.00 57.41	
100		ATOM	1291	CB	LYS	A	472	21.697 -16.777 13.713 1.00 58.74	
55		ATOM	1291	CG	LYS	A	472	20.683 -15.776 14.243 1.00 60.32	
(3)	35		1293	CD	LYS	A	472	19.271 -16.342 14.219 1.00 60.73	
W	33	MOTA MOTA	1294	CE	LYS	A	472	18.485 -15.909 15.449 1.00 61.78	
l.i.			1295	NZ	LYS	A	472	19.352 -15.788 16.658 1.00 60.09	
(3)		MOTA		C	LYS	A	472	23.662 -15.339 13.150 1.00 53.42	
		MOTA	1296	0	LYS	A	472	23.631 -14.120 12.978 1.00 50.87	
1	40	MOTA	1297	N	ASP	A	473	24.628 -15.949 13.830 1.00 47.52	
	40	ATOM	1298					25.732 -15.194 14.405 1.00 45.55	
		ATOM	1299	CA	ASP	A	473	26.613 -16.094 15.269 1.00 50.48	
		ATOM	1300	CB	ASP	A	473	26.380 -15.885 16.749 1.00 55.50	
		ATOM	1301	CG	ASP	A	473	25.272 -15.436 17.118 1.00 58.06	
		ATOM	1302	OD1	ASP	A	473	27.304 -16.170 17.541 1.00 59.81	
	45	ATOM	1303	OD2	ASP	A	473		
		ATOM	1304	С	ASP	A	473		
		MOTA	1305	0	ASP	A	473		
		ATOM	1306	N	HIS	A	474		
		ATOM	1307	CA	HIS	A	474		
	50	MOTA	1308	CB	HIS	A	474	27.429 -15.978 9.941 1.00 35.07	
		ATOM	1309		HIS	A	474	28.036 -15.523 8.653 1.00 37.36	
		MOTA	1310		HIS	Α	474	29.292 -15.113 8.355 1.00 38.86	
		ATOM	1311	ND1	HIS	A	474	27.322 -15.452 7.476 1.00 41.31	
		MOTA	1312	CE1	HIS	A	474	28.110 -15.020 6.509 1.00 40.86	
	55	ATOM	1313	NE2	HIS	A	474	29.311 -14.807 7.016 1.00 44.49	
		ATOM	1314	C	HIS	Α	474	26.749 -13.640 10.493 1.00 36.68	
		ATOM	1315	0	HIS	A	474	27.417 -12.676 10.132 1.00 36.48	
		ATOM	1316	N	ILE	A	475	25.422 -13.652 10.447 1.00 35.93	
		ATOM	1317		ILE	A	475	24.683 -12.499 9.963 1.00 36.21	
	60	ATOM	1318		ILE	A	475	23.174 -12.797 9.868 1.00 36.31	
		ATOM	1319		ILE	A	475	22.411 -11.527 9.513 1.00 38.19	
		ATOM	1320	CG1	ILE	Α	475	22.922 -13.874 8.813 1.00 36.97	
								172	

	-					_	455	21.528 -14.454 8.869 1.00 35.59
	5	ATOM	1321	CD1	ILE	Α	475	
		ATOM	1322	C	ILE	A	475	24.893 -11.322 10.907 1.00 35.34
		ATOM	1323	0	ILE	A	475	25.092 -10.189 10.471 1.00 33.20
		MOTA	1324	N	HIS	A	476	24.857 -11.596 12.206 1.00 35.95
		ATOM	1325	CA	HIS	A	476	25.031 -10.540 13.193 1.00 35.06
	10							24.681 -11.062 14.585 1.00 37.30
	10	MOTA	1326	CB	HIS	A	476	
		ATOM	1327	CG	HIS	A	476	
		ATOM	1328	CD2	HIS	Α	476	22.329 -10.051 15.017 1.00 43.93
		ATOM	1329	ND1	HIS	A	476	22.476 -12.230 14.968 1.00 45.60
		MOTA	1330	CE1	HIS	A	476	21.207 -11.928 15.177 1.00 47.56
	15	ATOM	1331	NE2	HIS	A	476	21.091 -10.613 15.211 1.00 46.21
	13	ATOM	1332	C	HIS	A	476	26.438 -9.966 13.170 1.00 35.40
				0	HIS	A	476	26.634 -8.774 13.415 1.00 35.45
		ATOM	1333				477	27.420 -10.805 12.862 1.00 34.07
		MOTA	1334	N	ARG	A		
		MOTA	1335	CA	ARG	A	477	
	20	ATOM	1336	CB	ARG	A	477	29.757 -11.506 12.605 1.00 41.04
		ATOM	1337	CG	ARG	A	477	29.800 -12.459 13.788 1.00 47.61
		ATOM	1338	CD	ARG	A	477	30.782 -13.599 13.557 1.00 55.67
		ATOM	1339	NE	ARG	A	477	31.780 -13.675 14.622 1.00 60.17
		ATOM	1340	CZ	ARG	A	477	32.780 -12.811 14.770 1.00 61.98
	25			NH1	ARG	A	477	32.918 -11.803 13.918 1.00 64.29
1100	25	MOTA	1341					33.643 -12.955 15.766 1.00 62.79
10		ATOM	1342	NH2	ARG	A	477	*
11		ATOM	1343	C	ARG	Α	477	
(12		ATOM	1344	0	ARG	A	477	29.462 -8.268 11.753 1.00 33.59
- Bade		ATOM	1345	N	VAL	A	478	28.369 -9.766 10.475 1.00 27.65
14	30	ATOM	1346	CA	VAL	Α	478	28.389 -8.930 9.280 1.00 27.07
		ATOM	1347	CB	VAL	A	478	27.658 -9.605 8.100 1.00 28.00
frak.		ATOM	1348	CG1	VAL	A	478	27.672 -8.678 6.890 1.00 25.83
1			1349	CG2	VAL	A	478	28.319 -10.933 7.761 1.00 31.66
24		MOTA					478	27.689 -7.610 9.584 1.00 26.92
(2) (J)		ATOM	1350	C	VAL	A		
Lif	35	ATOM	1351	0	VAL	A	478	
111		ATOM	1352	N	LEU	Α	479	26.499 -7.702 10.171 1.00 25.74
W C		ATOM	1353	CA	LEU	A	479	25.727 -6.516 10.530 1.00 27.97
100		MOTA	1354	CB	LEU	Α	479	24.474 -6.912 11.324 1.00 25.55
10		ATOM	1355	CG	LEU	Α	479	23.211 -7.229 10.517 1.00 29.01
10	40	ATOM	1356	CD1	LEU	A	479	22.056 -7.503 11.481 1.00 27.05
		ATOM	1357	CD2	LEU	Α	479	22.864 -6.063 9.584 1.00 24.92
			1358	C	LEU	A	479	26.592 -5.582 11.369 1.00 25.39
		ATOM				A	479	26.595 -4.370 11.158 1.00 27.39
		ATOM	1359	0	LEU			27.324 -6.158 12.320 1.00 26.04
		ATOM	1360	N	ASP	A	480	
	45	ATOM	1361	CA	ASP	A	480	
		ATOM	1362	CB	ASP	Α	480	28.878 -6.305 14.222 1.00 26.67
		ATOM	1363	CG	ASP	A	480	27.990 -6.602 15.417 1.00 31.02
		ATOM	1364	OD1	ASP	A	480	28.355 -7.505 16.198 1.00 31.50
		ATOM	1365	OD2	ASP	Α	480	26.935 -5.944 15.580 1.00 32.21
	50	ATOM	1366	C	ASP	A	480	29.283 -4.699 12.361 1.00 25.59
	50			0	ASP	A	480	29.672 -3.562 12.636 1.00 27.15
		ATOM	1367					29.767 -5.394 11.340 1.00 25.17
		ATOM	1368	N	LYS	A	481	==
		MOTA	1369	CA	LYS	Α	481	* · · · · · · · · · · · · · · · · ·
		MOTA	1370	CB	LYS	Α	481	31.306 -5.890 9.512 1.00 28.42
	55	MOTA	1371	CG	LYS	Α	481	32.158 -6.953 10.188 1.00 35.59
		ATOM	1372	CD	LYS	A	481	32.894 -7.799 9.157 1.00 41.21
		ATOM	1373	CE	LYS	A	481	33.883 -6.963 8.350 1.00 41.48
		ATOM	1374	NZ	LYS	A	481	34.954 -6.388 9.215 1.00 43.22
					LYS	A	481	30.260 -3.635 9.696 1.00 26.12
	60	ATOM	1375					30.979 -2.657 9.463 1.00 23.73
	60	MOTA	1376	0	LYS	A	481	
		ATOM	1377		ILE	A	482	
		MOTA	1378	CA	ILE	Α	482	28.421 -2.598 8.545 1.00 27.69
								1.50

	5	ATOM	1379	CB	ILE	А	482	27.066	-2.983	7.915	1.00	27.59
	,	ATOM	1380	CG2	ILE	A	482	26.470	-1.788	7.183	1.00	25.97
				CG1	ILE	A	482	27.274	-4.131	6.922	1.00	23.80
		ATOM	1381		ILE	A	482	26.000	-4.838	6.533	1.00	21.30
		ATOM	1382	CD1					-1.408	9.481	1.00	27.33
	10	ATOM	1383	C	ILE	A	482	28.253	-0.256	9.045	1.00	28.55
	10	ATOM	1384	0	ILE	A	482	28.312			1.00	25.03
		ATOM	1385	N	THR	A	483	28.046	-1.690			
		ATOM	1386	CA	THR	A	483	27.905	-0.632		1.00	23.62
		MOTA	1387	CB	THR	A	483	27.535	-1.192		1.00	22.18
		MOTA	1388	OG1	THR	A	483	26.181	-1.658		1.00	25.39
	15	ATOM	1389	CG2	THR	A	483	27.673	-0.111		1.00	25.84
		ATOM	1390	C	THR	Α	483	29.257		11.858	1.00	23.04
		ATOM	1391	0	THR	Α	483	29.331		11.846	1.00	23.55
		ATOM	1392	N	ASP	A	484	30.324	-0.714		1.00	22.24
		ATOM	1393	CA	ASP	A	484	31.674	-0.152	12.039	1.00	25.48
	20	ATOM	1394	CB	ASP	A	484	32.718	-1.273	12.107	1.00	26.88
		ATOM	1395	CG	ASP	A	484	32.629	-2.083	13.394	1.00	32.52
		ATOM	1396	OD1	ASP	A	484	32.002	-1.608	14.366	1.00	33.68
		ATOM	1397	OD2	ASP	A	484	33.185	-3.198	13.434	1.00	34.63
		ATOM	1398	C	ASP	Α	484	31.930	0.715	10.807	1.00	25.16
144	25	ATOM	1399	0	ASP	Α	484	32.481	1.812	10.905	1.00	26.05
1.2		ATOM	1400	N	THR	A	485	31.505	0.226	9.645	1.00	28.96
100		ATOM	1401	CA	THR	A	485	31.689	0.960	8.394	1.00	26.63
FU		ATOM	1402	CB	THR	A	485	31.124	0.166	7.197	1.00	26.12
ĮĮ.		ATOM	1403	OG1	THR	A	485	31.753	-1.123	7.132	1.00	24.30
justi	30	ATOM	1404	CG2	THR	A	485	31.381	0.907	5.898	1.00	23.31
1	30	ATOM	1405	C	THR	A	485	30.994	2.318	8.468	1.00	28.90
2 naix		ATOM	1405	Ö	THR	A	485	31.583	3.354	8.137	1.00	27.26
14		ATOM	1407	N	LEU	A	486	29.743	2.310	8.915	1.00	24.76
2)		ATOM	1407	CA	LEU	A	486	28.973	3.537	9.027	1.00	26.19
f ^{reb}	35		1409	CB	LEU	A	486	27.567	3.233	9.547	1.00	27.27
141	33	ATOM	1410	CG	LEU	A	486	26.508	2.921	8.486	1.00	23.50
		ATOM		CD1	LEU	A	486	25.210	2.550	9.183	1.00	22.03
2000		ATOM	1411 1412	CD2	LEU	A	486	26.309	4.128	7.577	1.00	21.35
:0		ATOM		CDZ	LEU	A	486	29.662	4.519	9.960	1.00	27.36
10	40	ATOM	1413		LEU		486	29.745	5.710	9.669	1.00	25.87
200	40	ATOM	1414	0		A	487	30.151		11.088	1.00	27.88
		ATOM	1415	N	ILE	A A	487	30.843		12.055	1.00	28.40
		ATOM	1416	CA	ILE			31.203		13.332	1.00	26.74
		ATOM	1417	CB	ILE	A A	487 487	32.255		14.154	1.00	27.54
	4.5	ATOM	1418	CG2	ILE			29.937		14.163	1.00	25.93
	45	ATOM	1419	CG1	ILE	A	487			14.624	1.00	23.42
		ATOM	1420	CD1	ILE	A	487	29.237		11.412	1.00	28.89
		ATOM	1421	С	ILE	A	487	32.125		11.602	1.00	29.85
		ATOM	1422	0	ILE	A	487	32.497			1.00	29.71
		MOTA	1423	N	HIS	A	488	32.791		10.649		
	50	MOTA	1424	CA	HIS	A	488	34.031	4.898	9.967	1.00	34.12
		ATOM	1425	CB	HIS	Α	488	34.585	3.691	9.207	1.00	36.61
		ATOM	1426	CG	HIS	A	488	35.799	3.997	8.385	1.00	42.74
		ATOM	1427	CD2	HIS	А	488	35.970	4.089	7.045	1.00	43.12
		ATOM	1428	ND1	HIS	Α	488	37.034	4.239	8.946	1.00	43.13
	55	ATOM	1429	CE1	HIS	A	488	37.913	4.466	7.987	1.00	43.40
		ATOM	1430	NE2	HIS	A	488	37.293	4.381	6.825	1.00	45.63
		ATOM	1431	C	HIS	A	488	33.799	6.051	8.998	1.00	32.74
		ATOM	1432	0	HIS	Α	488	34.577	7.004	8.955	1.00	31.06
		ATOM	1433	N	LEU	A	489	32.721	5.958	8.223	1.00	33.56
	60	ATOM	1434	CA	LEU	A	489	32.384	6.992	7.258	1.00	30.78
		ATOM	1435	CB	LEU	A	489	31.145	6.587	6.464	1.00	34.67
		ATOM	1436	CG	LEU	A	489	31.310	5.353	5.574	1.00	34.73
								174				

	5	ATOM	1437	CD1	LEU	A	489	29.945	4.856	5.125	1.00	33.21
		ATOM	1438	CD2	LEU	A	489	32.183	5.701	4.378	1.00	35.92
		ATOM	1439	C	LEU	A	489	32.124	8.320	7.954	1.00	33.97
		ATOM	1440	0	LEU	A	489	32.587	9.365	7.507	1.00	33.22
			1441	N	MET	A	490	31.387	8.274	9.058	1.00	31.33
	10	ATOM	1442	CA	MET	A	490	31.056	9.482	9.801	1.00	30.61
	10	ATOM				A	490	30.000		10.862	1.00	32.34
		ATOM	1443	CB	MET		490	28.607		10.289	1.00	30.71
		ATOM	1444	CG	MET	A		27.457		11.496	1.00	31.14
		ATOM	1445	SD	MET	A	490			10.418	1.00	30.36
		ATOM	1446	CE	MET	A	490	26.321			1.00	32.22
	15	ATOM	1447	C	MET	A	490	32.287	10.108			28.25
		ATOM	1448	0	MET	A	490	32.412	11.330		1.00	33.81
		ATOM	1449	N	ALA	A	491	33.184		10.949	1.00	39.92
		MOTA	1450	CA	ALA	A	491	34.407		11.585		37.22
		MOTA	1451	CB	ALA	A	491	35.168		12.185	1.00	
	20	ATOM	1452	C	ALA	A	491	35.275	10.445		1.00	42.68 45.32
		ATOM	1453	0	ALA	Α	491	35.865	11.487		1.00	45.32
		ATOM	1454	N	LYS	A	492	35.339	9.876	9.347	1.00	
		ATOM	1455	CA	LYS	A	492	36.122	10.440	8.248	1.00	44.80
		ATOM	1456	CB	LYS	Α	492	36.136	9.477	7.052	1.00	46.96
1.7	25	ATOM	1457	CG	LYS	A	492	37.490	8.840	6.744	1.00	47.20
1113		ATOM	1458	CD	LYS	A	492	37.390	7.830	5.595	1.00	45.71
10		ATOM	1459	CE	LYS	A	492	38.631	6.937	5.518	1.00	45.55
1,0		ATOM	1460	NZ	LYS	A	492	38.357	5.577	4.948	1.00	36.28
) min		ATOM	1461	C	LYS	A	492	35.534	11.780	7.809	1.00	45.61
4	30	ATOM	1462	0	LYS	A	492	36.227	12.604	7.215	1.00	46.18
14		ATOM	1463	N	ALA	Α	493	34.254	11.992	8.100	1.00	43.75
14		ATOM	1464	CA	ALA	A	493	33.590	13.238	7.728	1.00	42.42
81		ATOM	1465	CB	ALA	A	493	32.097	13.001	7.528	1.00	40.92
1004		ATOM	1466	C	ALA	A	493	33.816	14.305	8.796	1.00	41.78
	35	MOTA	1467	0	ALA	A	493	33.277	15.410	8.707	1.00	40.76
1,1		MOTA	1468	N	GLY	A	494	34.604	13.960	9.811	1.00	41.01
		MOTA	1469	CA	GLY	A	494	34.903	14.904		1.00	41.63
10		MOTA	1470	C	GLY	Α	494	33.857		11.965	1.00	41.18
0		ATOM	1471	0	GLY	Α	494	33.916		12.747	1.00	38.22
ibe	40	MOTA	1472	N	LEU	Α	495	32.905		12.043	1.00	39.53
		MOTA	1473	CA	LEU	A	495	31.876		13.068	1.00	38.91
		MOTA	1474	CB	LEU	Α	495	30.713		12.769	1.00	39.20
		MOTA	1475	CG	LEU	A	495	29.540		11.988	1.00	40.73
		ATOM	1476	CD1	LEU	A	495	29.976		10.553	1.00	37.80
	45	ATOM	1477	CD2	LEU	Α	495	28.349		12.026	1.00	40.94
		ATOM	1478	C	LEU	A	495	32.461		14.431	1.00	36.01
		ATOM	1479	0	LEU	A	495	33.347		14.544	1.00	34.85
		ATOM	1480	N	THR	A	496	31.979		15.459	1.00	37.52
		MOTA	1481	CA	THR	A	496	32.462		16,812	1.00	35.45
	50	ATOM	1482	CB	THR	A	496	31.925		17.829	1.00	37.55
		ATOM	1483	OG1	THR	A	496	30.498		17.908	1.00	32.93
		ATOM	1484	CG2	THR	Α	496	32.315		17.434	1.00	36.16
		ATOM	1485	C	THR	Α	496	31.933		17.210	1.00	35.67
		ATOM	1486	0	THR	A	496	31.081		16.521	1.00	34.34
	55	ATOM	1487	N	LEU	A	497	32.429		18.319	1.00	34.88
		ATOM	1488	CA	LEU	A	497	31.965		18.786	1.00	35.67
		ATOM	1489	CB	LEU	Α	497	32.689		20.074	1.00	41.10
		ATOM	1490	CG	LEU	A	497	33.714		19.896	1.00	45.27
		ATOM	1491	CD1	LEU	A	497	34.755		21.008	1.00	45.09
	60	ATOM	1492	CD2	LEU	A	497	32.988		19.884	1.00	47.77
		ATOM	1493	C	LEU	A	497	30.455		19.026	1.00	33.72
		ATOM	1494	0	LEU	A	497	29.712	10.350	18.534	1.00	33.20

	5	ATOM	1495	N	GLN	A	498	30.006	12.202 19.773	1.00	30.82
	,				GLN	A	498	28.586	12.348 20.062	1.00	31.47
		ATOM	1496	CA					13.566 20.951	1.00	30.51
		MOTA	1497	CB	GLN	A	498	28.344			34.38
		ATOM	1498	CG	GLN	A	498	26.894	13.796 21.341	1.00	
		ATOM	1499	CD	GLN	A	498	26.712	15.130 22.015	1.00	38.60
	10	ATOM	1500	OE1	GLN	A	498	27.363	16.112 21.686	1.00	42.92
		ATOM	1501	NE2	GLN	A	498	25.809	15.176 23.008	1.00	40.02
		ATOM	1502	C	GLN	A	498	27.776	12.476 18.773	1.00	30.47
		ATOM	1503	0	GLN	Α	498	26.682	11.927 18.665	1.00	30.85
		ATOM	1504	N	GLN	A	499	28.311	13.196 17.793	1.00	29.52
	15	ATOM	1505	CA	GLN	Α	499	27.603	13.362 16.524	1.00	30.24
		ATOM	1506	CB	GLN	Α	499	28.292	14.420 15.661	1.00	30.20
		ATOM	1507	CG	GLN	Α	499	28.135	15.840 16.191	1.00	31.60
		ATOM	1508	CD	GLN	Α	499	28.930	16.849 15.389	1.00	31.61
		ATOM	1509	OE1	GLN	A	499	29.956	16.518 14.795	1.00	30.66
	20	ATOM	1510	NE2	GLN	A	499	28.457	18.089 15.364	1.00	34.17
		ATOM	1511	C	GLN	A	499	27.529	12.047 15.753	1.00	29.40
		ATOM	1512	ō	GLN	A	499	26.567	11.793 15.032	1.00	30.04
		ATOM	1513	N	GLN	A	500	28.550	11.214 15.903	1.00	25.67
		ATOM	1514	CA	GLN	A	500	28.577	9.937 15.216	1.00	29.30
	25	ATOM	1515	CB	GLN	A	500	29.933	9.276 15.406	1.00	31.52
12	23	ATOM	1516	CG	GLN	A	500	31.012	9.839 14.508	1.00	33.05
423			1517	CD	GLN	A	500	32.371	9.370 14.930	1.00	34.84
il in		ATOM		OE1	GLN	A	500	32.612	8.194 15.141	1.00	36.47
133		ATOM	1518					33.301	10.324 15.082	1.00	38.25
n-fe	20	ATOM	1519	NE2	GLN	A	500	27.459	9.017 15.711	1.00	27.98
34	30	ATOM	1520	C	GLN	A	500			1.00	24.84
a si		ATOM	1521	0	GLN	A	500	26.700	8.469 14.908	1.00	26.20
2.1		ATOM	1522	N	HIS	A	501	27.357	8.864 17.029		27.63
31		ATOM	1523	CA	HIS	A	501	26.327	8.021 17.631	1.00	27.83
		ATOM	1524	CB	HIS	A	501	26.535	7.919 19.145		
141	35	ATOM	1525	CG	HIS	A	501	27.892	7.420 19.535	1.00	34.27
(4)		ATOM	1526	CD2	HIS	A	501	28.726	6.540 18.931	1.00	36.10
100		ATOM	1527	ND1	HIS	A	501	28.541	7.844 20.676	1.00	31.81
10		ATOM	1528	CE1	HIS	А	501	29.716	7.244 20.758	1.00	34.89
1D		ATOM	1529	NE2	HIS	А	501	29.854	6.448 19.712	1.00	37.46
1160	40	ATOM	1530	C	HIS	A	501	24.935	8.572 17.348	1.00	24.93
		MOTA	1531	0	HIS	Α	501	23.998	7.815 17.107	1.00	26.73
		MOTA	1532	N	GLN	A	502	24.796	9.892 17.379	1.00	22.79
		ATOM	1533	CA	GLN	Α	502	23.504	10.498 17.119	1.00	26.14
		ATOM	1534	CB	GLN	A	502	23.554	12.006 17.371	1.00	22.36
	45	ATOM	1535	CG	GLN	Α	502	23.460	12.378 18.848		26.19
		ATOM	1536	CD	GLN	Α	502	23.589	13.875 19.089	1.00	28.67
		ATOM	1537	OE1	GLN	A	502	23.632	14.663 18.149		28.40
		ATOM	1538	NE2	GLN	A	502	23.651	14.268 20.355		24.72
		ATOM	1539	C	GLN	Α	502	23.056	10.221 15.685	1.00	26.19
	50	ATOM	1540	0	GLN	A	502	21.913	9.822 15.453	1.00	24.09
		ATOM	1541	N	ARG	Α	503	23.955	10.429 14.727	1.00	24.88
		ATOM	1542	CA	ARG	A	503	23.630	10.196 13.326	1.00	25.25
		ATOM	1543	CB	ARG	A	503	24.772	10.668 12.418	1.00	27.63
		ATOM	1544	CG	ARG	A	503	24.432	10.563 10.932	1.00	28.75
	55	ATOM	1545	CD	ARG	Α	503	25.479	11.222 10.056	1.00	27.72
	55	ATOM	1546	NE	ARG	A	503	25.072	11.214 8.654		29.35
		ATOM	1547	CZ	ARG	A	503	24.279	12.126 8.105		25.84
		ATOM	1548	NH1	ARG	A	503	23.804	13.120 8.840		27.35
		ATOM	1549	NH2	ARG	A	503	23.962	12.044 6.820		30.63
	60	ATOM	1550	C	ARG	A	503	23.347	8.716 13.065		24.53
	00	ATOM	1551	0	ARG	A	503	22.425	8.375 12.321		25.90
		ATOM	1551	N	LEU	A	504	24.143	7.841 13.672		23.00
		ALON	T227	IA	الانتيا		504	21.113			

	5	ATOM	1553	CA	LEU	A	504	23.953	6.406	13.496	1.00	22.60
		ATOM	1554	CB	LEU	Α	504	24.971	5.621	14.323	1.00	25.43
		ATOM	1555	CG	LEU	Α	504	24.781	4.100	14.344	1.00	25.23
		ATOM	1556	CD1	LEU	A	504	25.166	3.505	12.991	1.00	28.52
		ATOM	1557	CD2	LEU	Α	504	25.627	3.495	15.444	1.00	22.14
	10	ATOM	1558	C	LEU	A	504	22.541	6.030	13.934	1.00	22.84
		ATOM	1559	0	LEU	Α	504	21.846	5.288	13.245	1.00	21.51
		ATOM	1560	N	ALA	Α	505	22.120	6.547	15.083	1.00	20.16
		ATOM	1561	CA	ALA	A	505	20.784	6.262	15.585	1.00	21.08
		ATOM	1562	CB	ALA	A	505	20.605	6.868	16.980	1.00	23.57
	15	ATOM	1563	C	ALA	A	505	19.738	6.832	14.628	1.00	20.20
	10	ATOM	1564	0	ALA	A	505	18.754	6.164	14.293	1.00	17.31
		ATOM	1565	N	GLN	Α	506	19.954	8.066	14.184	1.00	22.11
		ATOM	1566	CA	GLN	A	506	19.013	8.711	13.277	1.00	21.70
		ATOM	1567	CB	GLN	A	506	19.502	10.111	12.903	1.00	22.26
	20	ATOM	1568	CG	GLN	A	506	19.240	11.158		1.00	25.84
	20	ATOM	1569	CD	GLN	A	506	20.187	12.333		1.00	32.88
		ATOM	1570	OE1	GLN	A	506	20.704	12.614		1.00	31.23
		ATOM	1571	NE2	GLN	A	506	20.423	13.025		1.00	32.97
		ATOM	1572	C	GLN	A	506	18.813	7.881		1.00	23.57
	25	ATOM	1573	0	GLN	A	506	17.684	7.715		1.00	21.83
		ATOM	1574	N	LEU	A	507	19.905		11.474	1.00	19.98
10)	ATOM	1575	CA	LEU	A	507	19.827		10.263	1.00	22.03
11		ATOM	1576	CB	LEU	A	507	21.231	6.244	9.725	1.00	23.02
(7)		ATOM	1577	CG	LEU	A	507	22.026	7.457	9.225	1.00	25.80
g saw	30	ATOM	1578	CD1	LEU	A	507	23.371	6.994	8.713	1.00	27.67
543		ATOM	1579	CD2	LEU	A	507	21.264	8.176	8.130	1.00	25.62
la l		ATOM	1580	CDZ	LEU	A	507	19.090		10.496	1.00	22.35
14		ATOM	1581	ō	LEU	A	507	18.242	4.825	9.695	1.00	19.33
91		ATOM	1582	N	LEU	A	508	19.402		11.592	1.00	21.29
	35	ATOM	1583	CA	LEU	A	508	18.755		11.881	1.00	20.72
14.	33	ATOM	1584	CB	LEU	A	508	19.501		13.001	1.00	22.29
1.1		ATOM	1585	CG	LEU	A	508	20.977		12.678	1.00	24.70
\$186 \$125		ATOM	1586	CD1	LEU	A	508	21.642		13.814	1.00	21.37
ΝÜ		ATOM	1587	CD2	LEU	A	508	21.095		11.367	1.00	27.88
4		ATOM	1588	CDZ	LEU	A	508	17.279		12.239	1.00	19.14
	40	ATOM	1589	0	LEU	A	508	16.498		12.003	1.00	17.80
		ATOM	1590	N	LEU	A	509	16.895		12.815	1.00	19.23
		ATOM	1591	CA	LEU	A	509	15.495		13.173	1.00	20.14
		ATOM	1592	CB	LEU	A	509	15.347		13.999	1.00	20.28
	45	ATOM	1593	CG	LEU	A	509	15.710		15.479	1.00	21.35
	73	ATOM	1594	CD1	LEU	A	509	15.354		16.263	1.00	19.29
		ATOM	1595	CD2	LEU	A	509	14.989		16.038	1.00	20.84
		ATOM	1596	C	LEU	A	509	14.681		11.885	1.00	21.69
		ATOM	1597	0	LEU	A	509	13.493		11.854	1.00	22.40
	50		1598	N	ILE	A	510	15.343		10.815	1.00	20.22
	50	ATOM	1599	CA	ILE	A	510	14.710	5.397	9.508	1.00	20.40
		ATOM		CB	ILE	A	510	15.720	5.946	8.464	1.00	28.34
		ATOM	1600	CG2	ILE	A	510	15.208	5.710	7.056	1.00	32.54
		ATOM	1601 1602	CG1	ILE	A	510	15.265	7.438	8.696	1.00	28.23
	==	ATOM		CD1		A	510	14.789	8.189	9.288	1.00	33.16
	55	ATOM	1603		ILE		510	14.210	4.025	9.049	1.00	23.21
		MOTA	1604	C	ILE	A		13.120	3.906	8.474	1.00	21.16
		ATOM	1605	0	ILE	A	510	14.998	2.989	9.323	1.00	18.38
		ATOM	1606	N CA	LEU	A	511 511	14.633	1.634	8.917	1.00	20.10
	60	ATOM	1607	CB	LEU	A	511	15.754	0.656	9.267	1.00	21.69
	60	ATOM	1608	CG	LEU	A	511	17.128	1.022	8.692	1.00	26.03
		ATOM	1609		FEA	A	511	18.024	-0.206	8.724	1.00	22.68
		ATOM	1610	CD1	шеυ	A	OTT	10.024	0.200	0.724	1.00	

	5	ATOM	1611	CD2	LEU	A	511	16.996	1.544	7.267	1.00	26.00
		ATOM	1612	C	LEU	A	511	13.326	1.181	9.543	1.00	18.51
		ATOM	1613	0	LEU	Α	511	12.663	0.283	9.025	1.00	17.40
		ATOM	1614	N	SER	A	512	12.963		10.664	1.00	18.68
				CA	SER	A	512	11.718		11.331	1.00	18.67
	10	ATOM	1615							12.720	1.00	18.58
	10	ATOM	1616	CB	SER	A	512	11.661				
		ATOM	1617	OG	SER	A	512	10.315		13.165	1.00	27.92
		ATOM	1618	C	SER	A	512	10.572		10.464	1.00	18.43
		ATOM	1619	0	SER	A	512	9.584	1.296	10.236	1.00	13.91
		MOTA	1620	N	HIS	A	513	10.713	3.228	9.982	1.00	18.95
	15	ATOM	1621	CA	HIS	A	513	9.698	3.831	9.124	1.00	20.82
		ATOM	1622	CB	HIS	Α	513	10.013	5.315	8.894	1.00	24.36
		ATOM	1623	CG	HIS	Α	513	9.923	6.146	10.136	1.00	32.13
		ATOM	1624	CD2	HIS	A	513	8.863		10.734	1.00	35.29
		ATOM	1625	ND1	HIS	A	513	11.010		10.949	1.00	35.00
	20			CE1	HIS	A	513	10.624		11.995	1.00	34.67
	20	ATOM	1626							11.889	1.00	35.82
		MOTA	1627	NE2	HIS	A	513	9.326				
		ATOM	1628	C	HIS	A	513	9.650	3.079	7.790	1.00	19.08
		ATOM	1629	0	HIS	A	513	8.575	2.863	7.220	1.00	21.20
		ATOM	1630	N	ILE	Α	514	10.809	2.662	7.297	1.00	15.58
(ing	25	ATOM	1631	CA	ILE	Α	514	10.849	1.921	6.038	1.00	16.48
٠Ü		ATOM	1632	CB	ILE	A	514	12.312	1.678	5.576	1.00	20.09
IU.		ATOM	1633	CG2	ILE	A	514	12.349	0.602	4.499	1.00	19.55
		ATOM	1634	CG1	ILE	A	514	12.891	2.986	5.019	1.00	22.62
10		ATOM	1635	CD1	ILE	A	514	14.393	2.992	4.874	1.00	27.34
frei	30	ATOM	1636	C	ILE	A	514	10.112	0.590	6.210	1.00	16.40
4	50	ATOM	1637	Ö	ILE	A	514	9.364	0.164	5.328	1.00	17.91
inis.		ATOM	1638	N	ARG	A	515	10.301	-0.071	7.347	1.00	18.20
1				CA	ARG	A	515	9.585	-1.327	7.564	1.00	18.05
91		MOTA	1639						-1.980	8.889	1.00	18.36
E	2.5	ATOM	1640	CB	ARG	A	515	9.984				17.84
14.5	35	ATOM	1641	CG	ARG	A	515	9.173	-3.237	9.213	1.00	
8:3		MOTA	1642	CD	ARG	Α	515	9.823	-4.470	8.606	1.00	17.94
U		MOTA	1643	NE	ARG	A	515	11.038	-4.813	9.334	1.00	26.96
Ü		ATOM	1644	CZ	ARG	A	515	11.406	-6.051	9.641	1.00	25.13
40		ATOM	1645	NH1	ARG	Α	515	10.654	-7.080	9.281	1.00	23.49
184	40	ATOM	1646	NH2	ARG	A	515	12.511	-6.254	10.340	1.00	32.16
		ATOM	1647	C	ARG	A	515	8.089	-1.020	7.594	1.00	18.29
		ATOM	1648	0	ARG	A	515	7.275	-1.759	7.038	1.00	16.22
		MOTA	1649	N	HIS	Α	516	7.726	0.085	8.237	1.00	19.33
		ATOM	1650	CA	HIS	Α	516	6.317	0.441	8.330	1.00	17.78
	45	ATOM	1651	CB	HIS	A	516	6.126	1.702	9.166	1.00	16.84
	-13	ATOM	1652	CG	HIS	A	516	4.692	2.101	9.312	1.00	18.16
		ATOM	1653	CD2	HIS	A	516	3.967	3.061	8.691	1.00	21.17
								3.830		10.180	1.00	20.70
		ATOM	1654	ND1	HIS	A	516			10.180	1.00	21.52
		MOTA	1655	CE1	HIS	A	516	2.633				
	50	MOTA	1656	NE2	HIS	А	516	2.689	2.992	9.191	1.00	20.16
		ATOM	1657	C	HIS	A	516	5.708	0.659	6.954	1.00	16.63
		ATOM	1658	0	HIS	A	516	4.598	0.216	6.689	1.00	18.58
		ATOM	1659	N	MET	Α	517	6.438	1.334	6.073	1.00	15.29
		ATOM	1660	CA	MET	A	517	5.925	1.589	4.730	1.00	16.58
	55	ATOM	1661	CB	MET	A	517	6.837	2.576	4.002	1.00	18.66
		ATOM	1662	CG	MET	A	517	6.805	3.978	4.631	1.00	16.88
		ATOM	1663	SD	MET	A	517	7.670	5.243	3.701	1.00	24.08
		ATOM	1664	CE	MET	A	517	9.390	4.777	3.962	1.00	14.30
			1665	CE	MET	A	517	5.773	0.289	3.940	1.00	17.86
	60	ATOM						4.791	0.101	3.224	1.00	18.25
	60	ATOM	1666	0	MET	A	517			4.086	1.00	17.43
		MOTA	1667	N	SER	A	518	6.741	-0.610			
		MOTA	1668	CA	SER	A	518	6.697	-1.896	3.403	1.00	18.40

	5	ATOM	1669	CB	SER	А	518	7.974	-2.695	3.680	1.00	16.77
	,							7.834	-4.030	3.227	1.00	24.23
		MOTA	1670	OG	SER	A	518					
		ATOM	1671	C	SER	A	518	5.476	-2.695	3.854	1.00	17.91
		ATOM	1672	0	SER	Α	518	4.788	-3.295	3.030	1.00	18.97
		MOTA	1673	N	ASN	Α	519	5.204	-2.697	5.159	1.00	21.82
	10	ATOM	1674	CA	ASN	Α	519	4.047	-3.418	5.696	1.00	21.99
		ATOM	1675	CB	ASN	A	519	3.957	-3.257	7.216	1.00	23.24
		ATOM	1676	CG	ASN	Α	519	5.046	-4.011	7.957	1.00	31.14
		ATOM	1677	OD1	ASN	Α	519	5.585	-4.999	7.461	1.00	32.50
		ATOM	1678	ND2	ASN	Α	519	5.368	-3.545	9.163	1.00	29.10
	15	ATOM	1679	C	ASN	A	519	2.761	-2.871	5.079	1.00	23.76
		ATOM	1680	ō	ASN	A	519	1.902	-3.632	4.631	1.00	24.48
		ATOM	1681	N	LYS	A	520	2.627	-1.548	5.078	1.00	20.58
		ATOM	1682	CA	LYS	A	520	1.449	-0.900	4.512	1.00	25.49
					LYS	A	520	1.484	0.607	4.786	1.00	24.73
	20	ATOM	1683	CB						6.264	1.00	32.31
	20	ATOM	1684	CG	LYS	A	520	1.512	0.996			
		ATOM	1685	CD	LYS	Α	520	0.656	0.080	7.133	1.00	37.11
		ATOM	1686	CE	LYS	A	520	-0.787	0.547	7.181	1.00	41.56
		ATOM	1687	NZ	LYS	A	520	-1.560	-0.134	8.261	1.00	42.66
		MOTA	1688	C	LYS	A	520	1.380	-1.144	3.005	1.00	25.40
1000	25	ATOM	1689	0	LYS	А	520	0.316	-1.436	2.467	1.00	26.44
13		ATOM	1690	N	GLY	А	521	2.520	-1.021	2.332	1.00	22.88
14		ATOM	1691	CA	GLY	A	521	2.561	-1.236	0.897	1.00	21.53
109		ATOM	1692	C	GLY	A	521	2.177	-2.655	0.536	1.00	24.79
IQ Sub		ATOM	1693	0	GLY	Α	521	1.426	-2.878	-0.413	1.00	25.71
14.5	30	ATOM	1694	N	MET	A	522	2.696	-3.619	1.290	1.00	22.75
		ATOM	1695	CA	MET	Α	522	2.393	-5.027	1.058	1.00	23.40
2000		ATOM	1696	CB	MET	A	522	3.170	-5.898	2.042	1.00	25.74
1		ATOM	1697	CG	MET	A	522	3.396	-7.308	1.559	1.00	31.06
đi.		ATOM	1698	SD	MET	Α	522	4.572	-7.352	0.202	1.00	34.06
1.3	35	ATOM	1699	CE	MET	A	522	6.125	-7.229	1.113	1.00	29.28
1,1,3	33	ATOM	1700	C	MET	A	522	0.893	-5.281	1.218	1.00	26.49
U		ATOM	1701	0	MET	A	522	0.268	-5.920	0.361	1.00	25.47
100							523	0.321	-4.790	2.318	1.00	24.95
15		ATOM	1702	N	GLU	A						27.15
· O		ATOM	1703	CA	GLU	A	523	-1.110	-4.954	2.566	1.00	
140	40	ATOM	1704	CB	GLU	A	523	-1.555	-4.206	3.835	1.00	31.08
		ATOM	1705	CG	GLU	A	523	-0.830	-4.564	5.124	1.00	38.93
		ATOM	1706	CD	GLU	A	523	-1.153	-3.585	6.258	1.00	46.90
		ATOM	1707	OE1	GLU	Α	523	-2.225	-2.938	6.200	1.00	47.40
		MOTA	1708	OE2	GLU	Α	523	-0.337	-3.460	7.202	1.00	47.39
	45	ATOM	1709	C	GLU	А	523	-1.872	-4.368	1.381	1.00	26.10
		MOTA	1710	0	GLU	Α	523	-2.817	-4.964	0.882	1.00	24.25
		ATOM	1711	N	HIS	A	524	-1.449	-3.182	0.940	1.00	24.74
		MOTA	1712	CA	HIS	Α	524	-2.093	-2.505	-0.173	1.00	26.17
		ATOM	1713	CB	HIS	A	524	-1.481	-1.125	-0.379	1.00	24.64
	50	ATOM	1714	CG	HIS	А	524	-2.233	-0.278	-1.355	1.00	30.59
		MOTA	1715	CD2	HIS	А	524	-3.227		-1.172	1.00	32.15
		ATOM	1716	ND1	HIS	A	524	-2.008	-0.332		1.00	27.46
		ATOM	1717	CE1	HIS	A	524	-2.829		-3.326	1.00	34.58
		ATOM	1718	NE2	HIS	A	524	-3.580		-2.413	1.00	30.50
	55		1719	C	HIS	A	524	-1.996	-3.294		1.00	28.06
	33	ATOM						-2.976		-2.217	1.00	29.81
		ATOM	1720	0	HIS	A	524					
		MOTA	1721	N	LEU	A	525	-0.811	-3.824		1.00	27.07
		MOTA	1722	CA	LEU	A	525	-0.594	-4.601		1.00	29.30
		MOTA	1723	CB	LEU	A	525	0.865		-3.051	1.00	26.39
	60	ATOM	1724	CG	LEU	A	525	1.307		-4.321	1.00	29.34
		ATOM	1725	CD1	LEU	A	525	0.734		-5.562	1.00	29.61
		ATOM	1726	CD2	LEU	А	525	2.829	-5.769	-4.370	1.00	29.22

	5	ATOM	1727	C	LEU	A	525	-1.497 -5.822 -2.950 1.00 31.67
	,	ATOM		0	LEU	A	525	-2.128 -6.133 -3.957 1.00 32.45
		ATOM		N	TYR	A	526	-1.559 -6.512 -1.814 1.00 36.14
				CA	TYR	A	526	-2.397 -7.698 -1.696 1.00 40.36
		ATOM				A	526	-2.221 -8.350 -0.324 1.00 45.27
	10	MOTA		CB	TYR			-2.849 -9.722 -0.229 1.00 50.62
	10	MOTA		CG	TYR	A	526	
		ATOM		CD1	TYR	A	526	
		ATOM		CE1	TYR	A	526	
		ATOM		CD2	TYR	A	526	-4.188 -9.876 0.142 1.00 53.48
		ATOM		CE2	TYR	A	526	-4.781 -11.141 0.201 1.00 55.93
	15	MOTA	1737	CZ	TYR	Α	526	-4.029 -12.264 -0.113 1.00 56.60
		MOTA	1738	OH	TYR	A	526	-4.603 -13.515 -0.063 1.00 60.70
		ATOM	1739	C	TYR	A	526	-3.852 -7.298 -1.893 1.00 42.83
		MOTA	1740	0	TYR	A	526	-4.673 -8.094 -2.349 1.00 43.49
		ATOM	1741	N	SER	A	527	-4.158 -6.055 -1.543 1.00 41.55
	20	ATOM	1742	CA	SER	A	527	-5.503 -5.523 -1.686 1.00 44.04
		ATOM	1743	CB	SER	A	527	-5.606 -4.169 -0.979 1.00 43.47
		ATOM	1744	OG	SER	A	527	-6.954 -3.789 -0.786 1.00 47.51
		ATOM	1745	C	SER	A	527	-5.817 -5.356 -3.172 1.00 44.18
		ATOM		0	SER	A	527	-6.883 -5.757 -3.642 1.00 44.88
1199	25	ATOM		N	MET	A	528	-4.883 -4.755 -3.901 1.00 41.79
(13)		ATOM	1748	CA	MET	A	528	-5.047 -4.536 -5.331 1.00 44.04
10		ATOM	1749	CB	MET	A	528	-3.898 -3.679 -5.870 1.00 44.78
/U		ATOM	1750	CG	MET	A	528	-3.965 -2.206 -5.468 1.00 45.37
113		ATOM	1751	SD	MET	A	528	-5.652 -1.598 -5.273 1.00 51.83
int.	30	ATOM	1752	CE	MET	A	528	-5.553 -0.004 -6.044 1.00 46.61
14	50			C			528	-5.087 -5.871 -6.071 1.00 44.29
grass.		MOTA	1753		MET MET	A A	528	-5.689 -5.979 -7.137 1.00 44.02
302		MOTA	1754	0			529	-4.443 -6.883 -5.499 1.00 46.78
-		MOTA	1755	N	LYS	A		-4.413 -8.213 -6.099 1.00 51.28
O	25	MOTA	1756	CA	LYS	A	529	-3.550 -9.158 -5.261 1.00 50.87
M	35	ATOM	1757	CB	LYS	A	529	
111		ATOM	1758	CG	LYS	A	529	
13		ATOM	1759	CD	LYS	A	529	
·D		ATOM	1760	CE	LYS	A	529	
10		ATOM	1761	NZ	LYS	A	529	-2.420 -12.954 -4.402 1.00 53.22
759	40	ATOM	1762	C	LYS	Α	529	-5.829 -8.768 -6.182 1.00 54.27
		ATOM	1763	0	LYS	A	529	-6.325 -9.069 -7.266 1.00 55.50
		ATOM	1764	N	CYS	Α	530	-6.472 -8.901 -5.027 1.00 56.71
		ATOM	1765	CA	CYS	A	530	-7.833 -9.416 -4.961 1.00 58.35
		ATOM	1766	CB	CYS	A	530	-8.333 -9.380 -3.517 1.00 59.78
	45	MOTA	1767	SG	CYS	A	530	-7.289 -10.304 -2.358 1.00 63.19
		ATOM	1768	C	CYS	A	530	-8.766 -8.609 -5.858 1.00 59.36
		ATOM	1769	0	CYS	Α	530	-9.644 -9.169 -6.514 1.00 59.52
		ATOM	1770	N	LYS	A	531	-8.569 -7.293 -5.888 1.00 59.24
		ATOM	1771	CA	LYS	A	531	-9.390 -6.411 -6.713 1.00 60.14
	50	ATOM	1772	CB	LYS	Α	531	-9.158 -4.952 -6.317 1.00 58.92
		ATOM	1773	C	LYS	A	531	-9.073 -6.615 -8.195 1.00 61.48
		ATOM	1774	0	LYS	Α	531	-9.618 -5.928 -9.061 1.00 61.74
		ATOM	1775	N	ASN	A	532	-8.179 -7.561 -8.474 1.00 61.65
		ATOM	1776	CA	ASN	A	532	-7.783 -7.890 -9.840 1.00 61.60
	55	ATOM	1777	CB	ASN	A	532	-8.966 -8.518-10.581 1.00 62.28
	33		1778	CG	ASN	A	532	-8.750 -9.985-10.878 1.00 64.66
		ATOM			ASN	A	532	-8.344 -10.352-11.983 1.00 67.08
		ATOM	1779	OD1				-9.016 -10.836 -9.891 1.00 62.68
		ATOM	1780	ND2	ASN	A	532	-7.247 -6.710-10.648 1.00 59.75
	60	ATOM	1781	C	ASN	A	532	-7.247 -6.710-10.848 1.00 59.75 -7.487 -6.615-11.850 1.00 57.50
	60	ATOM	1782	0	ASN	A	532	
		MOTA	1783	N	VAL	A	533	
		ATOM	1784	CA	VAL	Α	533	
								180

	5	ATOM	1785	CB	VAL	A	533	-6.223	-3.371 -9.865	1.00	59.20
	5					A	533	-6.181	-2.163-10.785	1.00	59.21
		ATOM	1786	CG1	VAL					1.00	59.57
		ATOM	1787	CG2	VAL	A	533	-7.574	-3.467 -9.172		
		ATOM	1788	C	VAL	Α	533	-4.452	-4.767-10.907	1.00	57.86
		ATOM	1789	0	VAL	Α	533	-3.846	-3.874-11.499	1.00	60.56
	10	ATOM	1790	N	VAL	A	534	-3.852	-5.863-10.451	1.00	56.03
		ATOM	1791	CA	VAL	Α	534	-2.417	-6.063-10.621	1.00	54.11
		ATOM	1792	CB	VAL	Α	534	-1.767	-6.632 -9.341	1.00	54.02
		ATOM	1793	CG1	VAL	Α	534	-0.300	-6.950 -9.601	1.00	52.37
		ATOM	1794	CG2	VAL	Α	534	-1.900	-5.635 -8.200	1.00	55.70
	15	ATOM	1795	C	VAL	A	534	-2.089	-7.008-11.770	1.00	54.31
		ATOM	1796	ō	VAL	A	534	-2.519	-8.164-11.780	1.00	51.66
		ATOM	1797	N	PRO	A	535	-1.315	-6.527-12.755	1.00	53.54
		ATOM	1798	CD	PRO	A	535	-0.749	-5.172-12.874	1.00	54.28
		ATOM	1799	CA	PRO	A	535	-0.949	-7.373-13.893	1.00	53.24
	20			CB	PRO	A	535	0.011	-6.500-14.697	1.00	52.71
	20	ATOM	1800					-0.353	-5.102-14.319	1.00	53.19
		MOTA	1801	CG	PRO	A	535		-8.664-13.411	1.00	54.25
		MOTA	1802	C	PRO	A	535	-0.296		1.00	54.56
		MOTA	1803	0	PRO	Α	535	0.121	-8.768-12.254		
		ATOM	1804	N	LEU	A	536	-0.203	-9.645-14.299	1.00	53.63
	25	ATOM	1805	CA	LEU	A	536	0.382		1.00	53.11
		ATOM	1806	CB	LEU	A	536	-0.250	-12.046-14.763	1.00	51.88
	0 111	ATOM	1807	CG	LEU	A	536	-0.686	-13.256-13.938	1.00	51.83
	Ü	MOTA	1808	CD1	LEU	Α	536	-1.953	-12.917-13.173	1.00	49.51
1	at a	ATOM	1809	CD2	LEU	A	536	-0.905	-14.449-14.854	1.00	53.43
i	30	ATOM	1810	C	LEU	A	536	1.895	-10.990-14.081	1.00	52.58
-	2	MOTA	1811	0	LEU	A	536	2.414	-11.501-15.075	1.00	55.33
1	ui.	ATOM	1812	N	TYR	A	537	2.601	-10.462-13.087	1.00	48.72
		ATOM	1813	CA	TYR	A	537	4.057	-10.501-13.093	1.00	44.22
6	li paks	MOTA	1814	CB	TYR	Α	537	4.627	-9.134-12.709	1.00	44.52
3	35	ATOM	1815	CG	TYR	Α	537	4.331	-8.053-13.731	1.00	45.18
3	Ad	ATOM	1816	CD1	TYR	A	537	3.623	-6.905-13.376	1.00	43.77
1	J D	ATOM	1817	CE1	TYR	Α	537	3.334	-5.915-14.317	1.00	45.23
1	22	ATOM	1818	CD2	TYR	A	537	4.747	-8.187-15.058	1.00	46.91
-	0	ATOM	1819	CE2	TYR	A	537	4.462	-7.202-16.008	1.00	43.93
ě	₫ 40	ATOM	1820	CZ	TYR	A	537	3.757	-6.071-15.631	1.00	46.70
	40	ATOM	1821	OH	TYR	A	537	3.472	-5.097-16.565	1.00	48.35
		ATOM	1822	C	TYR	A	537		-11.562-12.056	1.00	41.29
		ATOM	1823	0	TYR	A	537		-11.319-10.856	1.00	41.82
		ATOM	1824	N	ASP	A	538		-12.748-12.540	1.00	40.34
	45			CA	ASP	A	538		-13.896-11.691	1.00	38.84
	43	ATOM	1825				538		-15.037-12.554	1.00	43.47
		ATOM	1826	CB	ASP	A			-15.531-13.566	1.00	47.67
		ATOM	1827	CG	ASP	A	538		-16.373-14.416	1.00	49.33
		MOTA	1828	OD1	ASP	A	538				
		ATOM	1829	OD2	ASP	A	538		-15.073-13.511	1.00	48.07
	50	ATOM	1830	C	ASP	A	538	5.991		1.00	37.28
		ATOM	1831	0	ASP	A	538		-13.964 -9.371	1.00	38.55
		ATOM	1832	N	LEU	A	539	7.196	-13.200-10.766	1.00	33.83
		ATOM	1833	CA	LEU	A	539	8.155	-12.959 -9.692	1.00	32.80
		ATOM	1834	CB	LEU	Α	539		-12.323-10.263	1.00	32.78
	55	ATOM	1835	CG	LEU	A	539	10.561	-12.031 -9.292	1.00	30.93
		ATOM	1836	CD1	LEU	A	539	10.913	-13.280 -8.492	1.00	33.81
		ATOM	1837	CD2	LEU	A	539	11.758	-11.538-10.077	1.00	25.92
		ATOM	1838	C	LEU	A	539	7.558	-12.050 -8.614	1.00	31.85
		ATOM	1839	Ō	LEU	А	539	7.590	-12.367 -7.423	1.00	25.63
	60	ATOM	1840	N	LEU	A	540	7.011	-10.917 -9.042	1.00	32.07
		ATOM	1841	CA	LEU	A	540	6.411	-9.976 -8.111	1.00	31.03
		ATOM	1842	CB	LEU	A	540	5.792	-8.800 -8.861	1.00	30.56
								181			

	5	ATOM	1843	CG	LEU	A	540	5.124	-7.774	-7.945	1.00	31.12
		ATOM	1844	CD1	LEU	A	540	6.092	-7.357	-6.838	1.00	29.76
		ATOM	1845	CD2	LEU	Α	540	4.693	-6.572	-8.762	1.00	30.85
		ATOM	1846	C	LEU	A	540	5.337	-10.660		1.00	34.55
		ATOM	1847	0	LEU	A	540	5.316	-10.522		1.00	31.60
1						A	541	4.446	-11.388		1.00	35.64
1	0	ATOM	1848	N	LEU				-12.101		1.00	37.84
		ATOM	1849	CA	LEU	Α	541	3.378				
		ATOM	1850	CB	LEU	A	541	2.452	-12.771		1.00	38.49
		ATOM	1851	CG	LEU	A	541		-11.932		1.00	39.80
		ATOM	1852	CD1	LEU	A	541	0.476	-11.476		1.00	40.02
1	15	ATOM	1853	CD2	LEU	A	541	1.713	-10.733	-9.485	1.00	40.48
		ATOM	1854	C	LEU	A	541	3.937	-13.147	-6.275	1.00	40.10
		ATOM	1855	0	LEU	A	541	3.472	-13.254	-5.137	1.00	42.72
		ATOM	1856	N	GLU	Α	542	4.929	-13.915	-6.723	1.00	38.45
		ATOM	1857	CA	GLU	A	542	5.535	-14.932	-5.868	1.00	39.59
2	20	ATOM	1858	CB	GLU	Α	542	6.738	-15.566	-6.564	1.00	41.73
_		ATOM	1859	CG	GLU	A	542	6.396	-16.327		1.00	48.34
		ATOM	1860	CD	GLU	A	542	6.931	-17.747		1.00	52.57
		ATOM	1861	OE1	GLU	A	542	8.049	-17.961		1.00	52.70
				OE2		A	542	6.230	-18.647		1.00	53.69
_		MOTA	1862		GLU			5.989	-14.299		1.00	39.94
100 4	25	ATOM	1863	C	GLU	A	542				1.00	40.99
10		ATOM	1864	0	GLU	A	542	5.567	-14.710			
143		MOTA	1865	N	MET	A	543		-13.287		1.00	38.29
10		MOTA	1866	CA	MET	A	543	7.380			1.00	38.11
fistly.		ATOM	1867	CB	MET	A	543		-11.408		1.00	37.34
NJ 3	30	ATOM	1868	CG	MET	Α	543	9.311	-11.797		1.00	40.59
Just .		ATOM	1869	SD	MET	Α	543		-12.223		1.00	45.64
1.1		ATOM	1870	CE	MET	A	543	12.014	-11.399	-5.151	1.00	42.61
		ATOM	1871	C	MET	A	543	6.287	-12.064	-2.581	1.00	37.94
81 2126-		ATOM	1872	0	MET	Α	543	6.413	-12.127	-1.358	1.00	39.20
四 :	35	ATOM	1873	N	LEU	A	544	5.218	-11.544	-3.175	1.00	39.44
in .		ATOM	1874	CA	LEU	Α	544	4.100	-11.013	-2.408	1.00	40.91
		ATOM	1875	CB	LEU	Α	544	3.087	-10.344	-3.341	1.00	39.88
22		ATOM	1876	CG	LEU	A	544	1.775	-9.905		1.00	42.70
		ATOM	1877	CD1	LEU	A	544	2.060	-8.886		1.00	37.35
10	40	ATOM	1878	CD2	LEU	A	544	0.854	-9.317		1.00	38.47
	10	ATOM	1879	C	LEU	A	544	3.420	-12.120		1.00	42.83
				0	LEU	A	544	2.957	-11.899		1.00	42.73
		ATOM	1880	N	ASP	A	545	3.367	-13.313		1.00	46.32
		ATOM	1881					2.746	-14.456		1.00	50.65
		ATOM	1882	CA	ASP	A	545				1.00	53.67
	45	ATOM	1883	CB	ASP	A	545	2.606	-15.617			
		ATOM	1884	CG	ASP	A	545	1.703	-15.278		1.00	57.35
		ATOM	1885	OD1	ASP	A	545	0.697			1.00	59.99
		ATOM	1886	OD2	ASP	A	545	1.999	-15.718		1.00	59.68
		ATOM	1887	C	ASP	A	545	3.559	-14.898		1.00	50.74
	50	ATOM	1888	0	ASP	A	545	3.004	-15.388	0.657	1.00	49.39
		ATOM	1889	N	ALA	Α	546	4.874	-14.723	-0.401	1.00	51.82
		ATOM	1890	CA	ALA	A	546	5.750	-15.095	0.702	1.00	53.12
		ATOM	1891	CB	ALA	A	546	7.180	-14.678	0.395	1.00	53.19
		ATOM	1892	C	ALA	A	546	5.269	-14.424	1.987	1.00	54.67
	55	ATOM	1893	0	ALA	A	546	5.476	-14.940	3.085	1.00	52.32
	22	ATOM	1894	N	HIS	A	547	4.622	-13.270	1.838	1.00	56.66
			1894	CA	HIS	A	547	4.102	-12.520	2.978	1.00	59.19
		ATOM						4.144	-11.017	2.684	1.00	56.70
		ATOM	1896	CB	HIS	A	547	4.144 5.489	-10.394	2.896	1.00	54.64
	c0	ATOM	1897	CG	HIS	A	547			2.199	1.00	53.92
,	60	MOTA	1898	CD2	HIS	A	547	6.644	-10.506			
		ATOM	1899	ND1	HIS	A	547	5.748	-9.514	3.925	1.00	52.17
		ATOM	1900	CE1	HIS	Α	547	7.004	-9.111	3.853	1.00	52.16

	5	ATOM	1901	NE2	HIS	Α	547	7.570 -9.698 2.814 1.00 51.90)
	-	ATOM	1902	C	HIS	Α	547	2.668 -12.940 3.306 1.00 62.77	/
		ATOM	1903	ō	HIS	A	547	1.842 -12.120 3.707 1.00 63.24	Ė
		ATOM	1904	N	ARG	A	548	2.381 -14.224 3.133 1.00 68.37	,
		ATOM	1905	CA	ARG	A	548	1.053 -14.758 3.411 1.00 72.75	
	10	ATOM	1906	CB	ARG	A	548	0.243 -14.864 2.113 1.00 73.73	
	10	ATOM	1907	CG	ARG	A	548	-1.149 -14.243 2.186 1.00 74.04	
		ATOM	1907	CD	ARG	A	548	-1.081 -12.728 2.297 1.00 74.50	
		ATOM	1908	NE	ARG	A	548	-2.305 -12.167 2.863 1.00 75.04	
			1910	CZ	ARG	A	548	-2.478 -10.880 3.149 1.00 75.59	
	1.5	ATOM				A	548	-1.506 -10.006 2.919 1.00 75.79	
	15	ATOM	1911	NH1 NH2	ARG	A	548	-3.627 -10.464 3.662 1.00 76.00	
		ATOM	1912		ARG			1.179 -16.133 4.061 1.00 74.94	
		ATOM	1913	C	ARG ARG	A	548 548	0.197 -16.697 4.549 1.00 75.19	
		ATOM	1914	0		A	549	2.398 -16.665 4.063 1.00 76.49	
	20	ATOM	1915	N CA	LEU	A A	549	2.669 -17.969 4.653 1.00 78.14	
	20	ATOM	1916	CB		A	549	2.971 -18.986 3.557 1.00 77.55	
		ATOM	1917		LEU		549	3.846 -17.870 5.619 1.00 79.13	
		ATOM	1918	C	LEU	A		4.892 -17.317 5.215 1.00 80.40	
		ATOM	1919	0	LEU	A	549	3.708 -18.341 6.769 1.00 79.46	
	25	ATOM	1920	OXT	LEU	A	549	5.390 -3.061 -6.139 1.00 21.38	
(mar)	25	HETATM	1921	CP9	DES	A	600	5.834 -1.989 -5.134 1.00 22.41	
10		HETATM	1922	CP8	DES	A	600		
11		HETATM	1923	CP7	DES	A	600	5.038 -0.714 -5.236 1.00 21.32 3.587 -0.864 -5.062 1.00 25.85	
(11)		HETATM	1924	CP6	DES	A	600	2.987 -0.978 -3.784 1.00 23.92	
g sales	20	HETATM	1925	CP1	DES	A	600	1.597 -1.150 -3.684 1.00 29.77	
34	30	HETATM	1926	CP2	DES	A	600		
1.4		HETATM	1927	CP3	DES	A	600	0.842 -1.214 -4.871 1.00 31.40 -0.506 -1.419 -4.824 1.00 33.36	
14		HETATM	1928	OP3	DES	A	600		
81		HETATM	1929	CP4	DES	A	600		
100	2.5	HETATM	1930	CP5	DES	A	600		
1,1	35	HETATM	1931	C7	DES	A	600	=	
T.		HETATM	1932	C6	DES	A	600		
1		HETATM	1933	C5	DES	A	600		
ıĎ.		HETATM	1934	C4	DES	A	600		
10		HETATM	1935	C3	DES	A	600		
140	40	HETATM	1936	03	DES	A	600		
		HETATM	1937	C2	DES	A	600		
		HETATM	1938	C1	DES	A	600		
		HETATM	1939	C8	DES	A	600		
		HETATM	1940	C9	DES	Α	600		
	45	HETATM	1941	CL	CL	A	601		
		ATOM	1942	CB	SER	В	305		
		ATOM	1943	C	SER	В	305		
		ATOM	1944	0	SER	В	305		
		ATOM	1945	N	SER	В	305	12.045 23.521 25.606 1.00 63.73	
	50	MOTA	1946	CA	SER	В	305	11.875 22.187 26.251 1.00 64.2	
		ATOM	1947		LEU	В	306	12.193 21.293 28.484 1.00 63.09	
		MOTA	1948	CA	LEU	В	306	12.884 21.133 29.757 1.00 60.98	
		MOTA	1949	CB	LEU	В	306	11.884 21.200 30.913 1.00 61.23	
		MOTA	1950		LEU	В	306	12.221 20.417 32.183 1.00 62.23	
	55	MOTA	1951		LEU	В	306	13.304 21.144 32.966 1.00 62.5 10.965 20.258 33.027 1.00 64.3	
		ATOM	1952		LEU	В	306		
		ATOM	1953		LEU	В	306	13.660 19.819 29.803 1.00 58.3	
		ATOM	1954		LEU	В	306	14.570 19.654 30.614 1.00 58.5	
		ATOM	1955		ALA	В	307	13.293 18.881 28.933 1.00 54.83	
	60	ATOM	1956		ALA	В	307	13.971 17.589 28.861 1.00 50.6	
		MOTA	1957		ALA	В	307	13.092 16.584 28.143 1.00 51.30 15.303 17.719 28.122 1.00 46.80	
		ATOM	1958	C	ALA	В	307		*
								183	

	5	ATOM	1959	0	ALA	В	307	16.196	16.885 28.274	1.00	45.62
		ATOM	1960	N	LEU	В	308	15.431	18.769 27.320	1.00	43.46
		MOTA	1961	CA	LEU	В	308	16.643	18.983 26.542	1.00	43.01
		ATOM	1962	CB	LEU	В	308	16.413	20.100 25.526	1.00	41.32
		ATOM	1963	CG	LEU	В	308	16.315	19.708 24.051	1.00	43.10
	10	ATOM	1964	CD1	LEU	В	308	15.942	18.239 23.903	1.00	40.51
	10	ATOM	1965	CD2	LEU	В	308	15.287	20.602 23.375	1.00	39.80
		ATOM	1966	C	LEU	В	308	17.874	19.297 27.385	1.00	42.11
		ATOM	1967	0	LEU	В	308	19.000	19.102 26.932	1.00	44.34
		ATOM	1968	N	SER	В	309	17.669	19.775 28.608	1.00	40.88
	15	ATOM	1969	CA	SER	В	309	18.796	20.100 29.475	1.00	42.79
	13			CB	SER	В	309	18.562	21.447 30.163	1.00	41.25
		ATOM	1970 1971	OG	SER	В	309	17.459	21.379 31.046	1.00	46.67
		ATOM ATOM	1971	C	SER	В	309	19.072	19.028 30.529	1.00	42.60
		ATOM	1972	0	SER	В	309	20.053	19.119 31.269	1.00	44.18
	20	ATOM	1973	N	LEU	В	310	18.217	18.012 30.596	1.00	39.44
	20		1975	CA	LEU		310	18.394	16.936 31.569	1.00	37.62
		ATOM		CB		B B	310	17.205	15.969 31.499	1.00	38.84
		ATOM	1976		LEU			16.216	15.873 32.668	1.00	42.43
		MOTA	1977	CG	LEU	В	310		17.219 33.355	1.00	42.43
	25	ATOM	1978	CD1	LEU	В	310	16.040 14.881	15.380 32.138	1.00	39.69
esal.	25	ATOM	1979	CD2	LEU	B B	310	19.691	16.174 31.285	1.00	34.11
143		ATOM	1980	C	LEU		310	20.111	16.070 30.139	1.00	34.41
IU.		MOTA	1981	0	LEU	В	310		15.662 32.326	1.00	34.04
10		MOTA	1982	N	THR	В	311	20.339 21.564	14.888 32.127	1.00	32.34
1.4	20	MOTA	1983	CA	THR	В	311		14.824 33.399	1.00	31.75
1	30	ATOM	1984	CB	THR	В	311	22.434 21.724	14.116 34.420	1.00	36.20
in.		MOTA	1985	OG1	THR	В	311	22.782	16.212 33.893	1.00	31.05
A.J		ATOM	1986	CG2	THR	В	311	21.145	13.460 31.790	1.00	32.37
97		ATOM	1987	C	THR	В	311		13.460 31.790	1.00	28.16
149	25	MOTA	1988	0	THR	В	311	19.967 22.106	12.628 31.396	1.00	33.23
1,4,5	35	ATOM	1989	N	ALA	B B	312 312	21.811	11.237 31.053	1.00	35.63
1,1		ATOM	1990	CA	ALA			23.077	10.527 30.577	1.00	34.00
0		ATOM	1991	CB	ALA	В	312	21.210	10.489 32.240	1.00	34.29
15		ATOM	1992	C	ALA	В	312	20.226	9.766 32.089	1.00	33.10
10	40	ATOM	1993	O N	ALA ASP	B B	312 313	21.800	10.665 33.419	1.00	33.10
	40	ATOM	1994			В	313	21.304	9.994 34.615	1.00	34.19
		MOTA	1995	CA	ASP			22.258	10.219 35.788	1.00	42.09
		MOTA	1996	CB	ASP	B B	313 313	23.494	9.358 35.700	1.00	44.87
		ATOM	1997	CG	ASP			24.586	9.858 36.040	1.00	51.57
	45	ATOM	1998	OD1 OD2	ASP	B B	313 313	23.377	8.184 35.290	1.00	46.79
	43	ATOM	1999		ASP		313	19.925	10.520 34.971	1.00	31.99
		MOTA	2000	C	ASP ASP	В	313	19.056	9.768 35.426	1.00	32.03
		ATOM	2001	0		B B	314	19.733	11.819 34.763	1.00	29.38
		ATOM	2002	N	GLN			18.458	12.457 35.046	1.00	29.73
	50	ATOM	2003	CA	GLN	В	314	18.562	13.966 34.832	1.00	32.88
	50	ATOM	2004	CB	GLN	В	314		14.732 36.085	1.00	36.47
		ATOM	2005	CG	GLN	В	314	18.970	16.208 35.815	1.00	36.76
		ATOM	2006	CD	GLN	В	314	19.213		1.00	38.79
		ATOM	2007	OE1	GLN	В	314	19.300	16.634 34.664	1.00	39.72
		ATOM	2008	NE2	GLN	В	314	19.327	16.995 36.880	1.00	29.11
	55	ATOM	2009	C	GLN	В	314	17.409	11.873 34.116		28.82
		ATOM	2010	0	GLN	В	314	16.274	11.620 34.522	1.00	
		ATOM	2011	N	MET	В	315	17.801	11.657 32.864	1.00	27.27
		ATOM	2012	CA	MET	В	315	16.900	11.079 31.872	1.00	30.41
		ATOM	2013	CB	MET	В	315	17.595	11.029 30.509		30.10
	60	ATOM	2014	CG	MET	В	315	16.787	10.345 29.421		38.02
		ATOM	2015	SD	MET	В	315	15.252	11.220 29.065	1.00	41.12
		ATOM	2016	CE	MET	В	315	15.890	12.835 28.611	1.00	39.32
								10/			

5	ATOM .	2017	C	MET	В	315	16.490	9.665 32.311	1.00	27.99
,										26.60
										27.26
										24.54
										26.22
10										29.81
10										29.75
										27.22
										25.55
										24.40
15										27.63
										31.68
										39.97
	ATOM									26.73
										25.65
20										24.19
										24.17
										21.44
	ATOM									21.63
										20.25
25	ATOM									23.37
	ATOM									25.42
	ATOM									22.03
	ATOM									20.71
	ATOM									23.60
30										23.82
										27.26
										28.91
										26.58
										26.73
35										26.87
										26.15
										28.04
										26.96
										29.19
40	ATOM									26.66
										29.72
										31.36
										36.60
										46.11
45										46.64
										45.98
										28.29
										27.19
										28.34
50										25.55
										24.11
										22.80
										24.54
										20.16
55										21.44
	MOTA									23.72
	ATOM									23.58
	ATOM	2070								25.23
	ATOM	2071								21.74
60	ATOM									25.49
	MOTA									22.35
	ATOM	2074	0	GLU	В	323	5.409	2.926 35.951	1.00	22.34
	30	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	ATOM 2018 ATOM 2019 ATOM 2020 ATOM 2021 10 ATOM 2023 ATOM 2023 ATOM 2026 ATOM 2028 ATOM 2030 ATOM 2030 ATOM 2031 ATOM 2031 ATOM 2032 ATOM 2036 ATOM 2036 ATOM 2036 ATOM 2036 ATOM 2036 ATOM 2036 ATOM 2037 ATOM 2036 ATOM 2040 ATOM 2040 ATOM 2041 ATOM 2041 ATOM 2042 ATOM 2043 ATOM 2045 ATOM 2045 ATOM 2046 ATOM 2045 ATOM 2046 ATOM 2046 ATOM 2055 ATOM 2056 ATOM 2066 ATOM 2067 ATOM 2068 ATOM 2066 ATOM 2067 ATOM 2068 ATOM 2068 ATOM 2066 ATOM 2068 ATOM 2069 ATOM 2060 ATOM 2070 ATOM 2070 ATOM 2070	ATOM 2018 O ATOM 2020 CA ATOM 2021 CB ATOM 2021 CG1 ATOM 2022 CG1 ATOM 2022 CG1 ATOM 2024 C ATOM 2025 O ATOM 2025 O ATOM 2026 CG ATOM 2026 CG ATOM 2027 CA ATOM 2026 CG ATOM 2027 CA ATOM 2030 C ATOM 2031 C ATOM 2031 C ATOM 2031 C ATOM 2032 N ATOM 2033 CA ATOM 2034 CB ATOM 2035 C ATOM 2035 C ATOM 2036 CA ATOM 2036 CA ATOM 2036 CG ATOM 2037 N ATOM 2036 CG ATOM 2040 CG ATOM 2040 CG ATOM 2040 CG ATOM 2040 CG ATOM 2041 CD2 ATOM 2041 CD2 ATOM 2042 CD2 ATOM 2043 C ATOM 2044 CD2 ATOM 2045 N ATOM 2046 CG ATOM 2047 CB ATOM 2046 CG ATOM 2047 CB ATOM 2048 CG ATOM 2048 CG ATOM 2048 CG ATOM 2049 CD1 ATOM 2049 CD1 ATOM 2046 CG ATOM 2047 CB ATOM 2046 CG ATOM 2047 CB ATOM 2046 CG ATOM 2055 CB ATOM 2055 CB ATOM 2055 CB ATOM 2056 CG ATOM 2056 CG ATOM 2056 CG ATOM 2056 CG ATOM 2057 CD ATOM 2056 CG ATOM 2066 CG ATOM 2066 CG ATOM 2066 CG ATOM 2067 CD ATOM 2067 CG ATOM 2068 CB ATOM 2067 CG ATOM 2070 CD ATOM 2070 CD ATOM 2070 CD ATOM 2070 CD	ATOM 2018 O MET ATOM 2019 N VAL ATOM 2021 CB VAL ATOM 2021 CB VAL ATOM 2022 CG1 VAL ATOM 2022 CG1 VAL ATOM 2024 C VAL ATOM 2025 O VAL ATOM 2026 N SER ATOM 2026 N SER ATOM 2027 CA SER ATOM 2028 CB SER ATOM 2030 C SER ATOM 2030 C SER ATOM 2031 O SER ATOM 2031 C SER ATOM 2031 C SER ATOM 2032 N ALA ATOM 2031 C SER ATOM 2032 N ALA ATOM 2034 C BAL ATOM 2034 C BAL ATOM 2035 C ALB ATOM 2036 C BAL ATOM 2037 N LEU ATOM 2038 CA LEU ATOM 2038 CA LEU ATOM 2039 C BLEU ATOM 2040 CG LEU ATOM 2040 CG LEU ATOM 2041 CD LEU ATOM 2041 CD LEU ATOM 2042 CD2 LEU ATOM 2043 C LEU ATOM 2044 CB LEU ATOM 2045 N LEU ATOM 2046 CA LEU ATOM 2047 CB LEU ATOM 2048 CG LEU ATOM 2048 CG LEU ATOM 2049 CD LEU ATOM 2048 CG LEU ATOM 2048 CG LEU ATOM 2049 CD LEU ATOM 2049 CD LEU ATOM 2040 CB LEU ATOM 2040 CB LEU ATOM 2041 CB LEU ATOM 2045 N LEU ATOM 2045 N LEU ATOM 2045 N LEU ATOM 2045 N LEU ATOM 2046 CA LEU ATOM 2047 CB LEU ATOM 2048 CG LEU ATOM 2048 CG LEU ATOM 2050 CD2 LEU ATOM 2051 C LEU ATOM 2051 C LEU ATOM 2052 C ASP ATOM 2054 CR ASP ATOM 2055 CB ASP ATOM 2056 CB ASP ATOM 2066 CB ASP ATOM 2066 CB ASP ATOM 2067 CA GBU ATOM 2068 CB GEU ATOM 2067 CD GEU ATOM 2070 CD GEU ATOM 2070 CD GEU ATOM 2070 CD CB CEU	ATOM 2018 O MET B ATOM 2019 N VAL B ATOM 2020 CA VAL B ATOM 2021 CB VAL B ATOM 2021 CG VAL B ATOM 2022 CG1 VAL B ATOM 2023 CG2 VAL B ATOM 2024 C VAL B ATOM 2025 O VAL B ATOM 2026 N SER B ATOM 2027 CA SER B ATOM 2028 CB SER B ATOM 2029 OG SER B ATOM 2020 C SER B ATOM 2021 C SER B ATOM 2022 C C VAL B ATOM 2025 N SER B ATOM 2020 C SER B ATOM 2021 C SER B ATOM 2031 C SER B ATOM 2031 C SER B ATOM 2032 C ALA B ATOM 2035 C ALA B ATOM 2035 C ALA B ATOM 2035 C ALA B ATOM 2036 C LEU B ATOM 2037 N LEU B ATOM 2038 CA LEU B ATOM 2039 CB LEU B ATOM 2040 CG LEU B ATOM 2041 CD1 LEU B ATOM 2041 CD1 LEU B ATOM 2042 CD2 LEU B ATOM 2043 C LEU B ATOM 2045 N LEU B ATOM 2045 N LEU B ATOM 2045 N LEU B ATOM 2045 C LEU B ATOM 2045 C LEU B ATOM 2045 C LEU B ATOM 2046 CA LEU B ATOM 2045 C LEU B ATOM 2046 CA LEU B ATOM 2047 CB LEU B ATOM 2048 CG LEU B ATOM 2048 CG LEU B ATOM 2049 CD1 LEU B ATOM 2049 CD1 LEU B ATOM 2049 CD1 LEU B ATOM 2050 CD2 LEU B ATOM 2050 CD2 LEU B ATOM 2051 C LEU B ATOM 2050 CD2 ASP B ATOM 2061 N ALA B ATOM 2050 CD2 ASP B ATOM 2050 CD2 ASP B ATOM 2061 CA ALA B ATOM 2050 CD2 ASP B ATOM 2062 CA ALA B ATOM 2050 CD2 ASP B ATOM 2063 CB ALA B ATOM 2065 CB ASP B ATOM 2066 N ASP B ATOM 2066 C ALA B ATOM 2067 CA ALA B ATOM 2068 CB ALA B ATOM 2068 CB ALA B ATOM 2069 CG GLU B ATOM 2069 CG GLU B ATOM 2069 CG GLU B ATOM 2060 CG GLU B ATOM 2070 CD GLU B	ATOM 2018 O MET B 315 ATOM 2019 N VAL B 316 ATOM 2021 CA VAL B 316 ATOM 2021 CB VAL B 316 ATOM 2022 CG1 VAL B 316 ATOM 2024 CV VAL B 316 ATOM 2025 O VAL B 316 ATOM 2026 CB SER B 317 ATOM 2027 CA SER B 317 ATOM 2023 CB SER B 317 ATOM 2030 C SER B 317 ATOM 2031 C SER B 317 ATOM 2031 C SER B 317 ATOM 2032 N ALA B 318 ATOM	ATOM 2018 O MET B 315 15.302 ATOM 2019 N VAL B 316 17.481 ATOM 2020 CA VAL B 316 17.229 ATOM 2021 CB VAL B 316 18.554 ATOM 2022 CG1 VAL B 316 18.574 ATOM 2022 CG2 VAL B 316 18.579 ATOM 2024 CV VAL B 316 15.397 ATOM 2024 CA SER B 317 16.601 ATOM 2027 CA SER B 317 16.358 ATOM 2030 C SER B 317 16.358 ATOM 2030 C SER B 317 16.368 ATOM 2031 C ALA B 318 12.786 ATOM	ATOM 2019 O MET B 315 15.302 9.351 32.396 ATOM 2019 N VAL B 316 17.481 8.823 32.598 ATOM 2020 CA VAL B 316 17.429 7.447 33.027 ATOM 2021 CB VAL B 316 18.554 6.708 33.351 10 ATOM 2022 CG1 VAL B 316 18.572 5.404 34.096 ATOM 2023 CG2 VAL B 316 18.272 5.404 34.096 ATOM 2025 O VAL B 316 19.302 6.410 32.074 ATOM 2025 O VAL B 316 15.397 6.579 34.318 ATOM 2026 N SER B 317 16.601 8.243 35.242 ATOM 2027 CA SER B 317 16.601 8.243 35.242 ATOM 2028 CB SER B 317 16.99 8.268 36.460 ATOM 2020 OC SER B 317 17.492 8.771 38.112 ATOM 2021 O SER B 317 14.346 8.600 36.154 ATOM 2031 O SER B 317 14.346 8.600 36.154 ATOM 2032 N ALA B 318 14.135 9.634 35.342 ATOM 2033 CA ALA B 318 12.786 10.049 34.969 ATOM 2034 CB ALA B 318 12.786 10.049 34.969 ATOM 2035 C ALA B 318 12.038 8.890 34.306 ATOM 2036 C ALA B 318 12.038 8.890 34.306 ATOM 2037 N LEU B 319 12.695 8.225 33.364 ATOM 2038 CA ALA B 318 12.038 8.890 34.306 ATOM 2039 CB LEU B 319 12.098 7.102 32.652 ATOM 2037 N LEU B 319 12.098 7.102 32.652 ATOM 2039 CB LEU B 319 13.050 6.635 31.548 ATOM 2039 CB LEU B 319 13.050 6.635 31.548 ATOM 2040 CG LEU B 319 13.050 6.635 31.548 ATOM 2040 CG LEU B 319 13.050 6.635 31.548 ATOM 2040 CG LEU B 319 13.050 6.635 31.548 ATOM 2040 CG LEU B 319 13.050 6.635 31.548 ATOM 2040 CG LEU B 319 13.050 6.635 31.548 ATOM 2040 CG LEU B 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B 316 18.554 6.708 33.351 1.00 ATOM 2023 CG2 VAL B 316 18.272 5.404 43.096 1.00 ATOM 2024 CC VAL B 316 18.272 5.404 43.096 1.00 ATOM 2025 O VAL B 316 16.326 7.389 34.258 1.00 ATOM 2026 N SER B 316 16.326 7.389 34.258 1.00 ATOM 2027 CA SER B 317 16.601 8.243 35.242 1.00 ATOM 2028 CB SER B 317 15.799 8.268 36.460 1.00 ATOM 2029 OG SER B 317 16.436 8.243 35.242 1.00 ATOM 2030 C SER B 317 17.492 8.771 38.112 1.00 ATOM 2031 O SER B 317 17.492 8.771 38.112 1.00 ATOM 2031 O SER B 317 14.346 8.600 36.154 1.00 ATOM 2032 N ALA B 318 14.135 9.634 35.342 1.00 ATOM 2033 CA ALA B 318 14.135 9.634 35.342 1.00 ATOM 2033 CA ALA B 318 12.880 11.250 34.022 1.00 ATOM 2035 C ALA B 318 12.038 8.890 34.306 1.00 ATOM 2036 C ALA B 318 12.038 8.890 34.306 1.00 ATOM 2037 N LEU B 319 12.098 7.102 33.648 1.00 ATOM 2038 CA LEU B 319 12.695 8.225 33.364 1.00 ATOM 2039 CB LEU B 319 12.695 8.225 33.364 1.00 ATOM 2039 CB LEU B 319 13.050 6.635 31.548 1.00 ATOM 2036 CA LEU B 319 13.050 6.635 31.548 1.00 ATOM 2040 CG LEU 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	5	ATOM	2075	N	PRO	В	324	4.986	2.165 33.880	1.00	19.10
	,	ATOM		CD	PRO	В	324	5.286	1.806 32.483	1.00	19.11
				CA	PRO	В	324	3.607	1.839 34.242	1.00	22.04
		ATOM				В	324	2.919	1.658 32.893	1.00	21.96
		MOTA		CB	PRO			4.015	1.137 32.015	1.00	24.13
		ATOM		CG	PRO	В	324		0.556 35.060	1.00	23.44
	10	ATOM		C	PRO	В	324	3.619	-0.200 35.028	1.00	22.20
		MOTA		0	PRO	В	324	4.590			
		ATOM		N	PRO	В	325	2.540	0.287 35.801	1.00	24.88
		ATOM		CD	PRO	В	325	1.299	1.068 35.945		26.67
		ATOM	2084	CA	PRO	В	325	2.520	-0.940 36.603	1.00	25.10
	15	ATOM	2085	CB	PRO	В	325	1.394	-0.691 37.595	1.00	27.09
		ATOM	2086	CG	PRO	В	325	0.448	0.205 36.854	1.00	26.87
		ATOM	2087	C	PRO	В	325	2.270	-2.192 35.776		25.77
		ATOM	2088	0	PRO	В	325	1.853	-2.118 34.617	1.00	21.69
		ATOM		N	ILE	В	326	2.538	-3.344 36.379	1.00	24.05
	20	ATOM	2090	CA	ILE	В	326	2.301	-4.620 35.722	1.00	22.51
		ATOM	2091	CB	ILE	В	326	3.303	-5.688 36.185	1.00	25.81
		ATOM	2092	CG2	ILE	В	326	3.011	-7.018 35.481	1.00	23.78
		ATOM	2093	CG1	ILE	В	326	4.729	-5.209 35.900	1.00	25.75
		ATOM	2094	CD1	ILE	В	326	5.241	-5.585 34.533		27.78
	25	ATOM	2095	C	ILE	В	326	0.893	-5.020 36.149		23.63
123	23	ATOM	2096	0	ILE	В	326	0.632	-5.231 37.332		24.81
13		ATOM	2097	N	LEU	В	327	-0.018	-5.104 35.188		19.44
			2098	CA	LEU	В	327	-1.399	-5.437 35.493		17.03
1,15		ATOM	2098	CB	LEU	В	327	-2.336	-4.747 34.493		18.39
Tu-à	20	ATOM			LEU	В	327	-2.201	-3.216 34.373		20.69
1	30	MOTA	2100	CG CD1	LEU	В	327	-3.245	-2.679 33.406		14.87
good-		ATOM	2101				327	-2.384	-2.570 35.742		14.39
Nagi		ATOM	2102	CD2	LEU	В		-1.662	-6.928 35.499		19.87
21		ATOM	2103	C	LEU	В	327	-0.854	-7.722 35.014		20.90
100	2.5	MOTA	2104	0	LEU	В	327		-7.300 36.06		20.92
(1) (u)	35	MOTA	2105	N	TYR	В	328	-2.803	-8.692 36.135		21.79
1,1		MOTA	2106	CA	TYR	В	328	-3.202			22.91
4119		ATOM	2107	CB	TYR	В	328	-3.658	-9.050 37.550		24.60
		MOTA	2108	CG	TYR	В	328	-2.515	-9.376 38.468		
10		ATOM	2109	CD1	TYR	В	328	-2.118	-10.696 38.67		25.93
- Ar	40	MOTA	2110	CE1	TYR	В	328	-1.034	-11.000 39.498		28.10
		MOTA	2111	CD2	TYR	В	328	-1.802	-8.362 39.103		29.46
		MOTA	2112	CE2	TYR	В	328	-0.716	-8.654 39.926		35.30
		ATOM	2113	CZ	TYR	В	328	-0.338	-9.973 40.11		32.59
		ATOM	2114	OH	TYR	В	328	0.739	-10.257 40.923		37.24
	45	MOTA	2115	C	TYR	В	328	-4.336	-8.944 35.16		22.25
		MOTA	2116	0	TYR	В	328	-5.115	-8.039 34.849		19.77
		ATOM	2117	N	SER	В	329	-4.420	-10.180 34.69		25.81
		MOTA	2118	CA	SER	В	329	-5.480	-10.571 33.78	7 1.00	29.39
		ATOM	2119	CB	SER	В	329	-5.002	-11.710 32.88	7 1.00	27.65
	50	ATOM	2120	OG	SER	В	329	-6.091	-12.329 32.23	1.00	28.98
		MOTA	2121	C	SER	В	329	-6.625	-11.042 34.67	1.00	33.17
		ATOM	2122	0	SER	В	329	-6.453	-11.157 35.88	3 1.00	32.52
		MOTA	2123	N	GLU	В	330	-7.792	-11.289 34.08	1.00	38.75
		MOTA	2124	CA	GLU	В	330	-8.930	-11.776 34.85	1.00	44.91
	55	ATOM	2125	CB	GLU	В	330	-10.134	-11.999 33.95	1.00	45.63
	55	ATOM	2126	C	GLU	В	330	-8.493	-13.093 35.49		48.62
		ATOM	2127	0	GLU	В	330	-7.739	-13.851 34.88		52.37
		ATOM	2127	N	TYR	В	331		-13.366 36.70		51.75
			2128	CA	TYR	В	331	-8.575	-14.596 37.39		55.25
	60	ATOM	2129	CB	TYR	В	331	-8.538	-14.365 38.91		53.04
	ou	MOTA		CG	TYR	В	331	-9.769			50.70
		ATOM	2131 2132	CD1	TYR	В	331		-14.400 39.85		47.09
		ATOM	2132	CDI	TIK	ь	J J L	10.000	11.400 33.03		

5 ATOM 2133 CE1 TYR B 331 -12.035 -13.762 40.292 1.0 ATOM 2134 CD2 TYR B 331 -10.993 -11.625 39.913 1.0 ATOM 2135 CE2 TYR B 331 -10.993 -11.625 39.913 1.0 ATOM 2136 CZ TYR B 331 -12.086 -12.376 40.314 1.0 ATOM 2137 OH TYR B 331 -12.086 -12.376 40.314 1.0 ATOM 2138 C TYR B 331 -9.528 -15.743 37.075 1.0 ATOM 2138 C TYR B 331 -9.528 -15.743 37.075 1.0 ATOM 2140 N ASP B 331 -9.528 -15.743 37.075 1.0 ATOM 2141 CA ASP B 332 -9.704 -18.124 36.490 1.0 ATOM 2142 CB ASP B 332 -9.704 -18.124 36.490 1.0 ATOM 2143 CG ASP B 332 -10.637 -17.895 35.290 1.0 ATOM 2144 OD1 ASP B 332 -11.723 -18.953 35.200 1.0 ATOM 2145 OD2 ASP B 332 -11.723 -18.953 35.200 1.0 ATOM 2146 C ASP B 332 -12.876 -18.602 34.866 1.0 ATOM 2147 O ASP B 332 -12.876 -18.602 34.866 1.0 ATOM 2146 C ASP B 332 -8.707 -19.227 36.153 1.0 ATOM 2146 C ASP B 333 -9.808 -20.690 37.875 1.0 ATOM 2146 C ASP B 333 -9.808 -20.690 37.875 1.0 ATOM 2146 D PRO B 333 -9.808 -20.690 37.875 1.0 ATOM 2150 CA PRO B 333 -9.808 -20.690 37.875 1.0 ATOM 2151 CB PRO B 333 -7.901 -21.503 36.596 1.0 ATOM 2155 C PRO B 333 -7.901 -21.503 36.596 1.0 ATOM 2155 C THR B 334 -9.309 -22.340 35.351 1.0 ATOM 2156 CA THR B 334 -9.309 -22.071 38.347 1.0 ATOM 2157 CB THR B 334 -9.649 -22.832 33.475 1.0 ATOM 2156 CA THR B 334 -9.649 -22.832 33.475 1.0 ATOM 2156 CA THR B 334 -9.649 -22.832 33.475 1.0 ATOM 2157 CB THR B 334 -11.065 -22.347 32.975 1.0 ATOM 2160 C THR B 334 -1.10.65 -22.477 32.975 1.0 ATOM 2161 O THR B 334 -1.10.65 -22.477 32.975 1.0 ATOM 2162 N ARG B 335 -6.302 -22.298 29.298 1.0 ATOM 2167 N PRO B 336 -7.938 -25.227 30.769 1.0 ATOM 2167 N PRO B 336 -7.938 -25.227 30.769 1.0 ATOM 2167 N PRO B 336 -7.937 -24.194 29.884 1.0 ATOM 2167 C PRO B 336 -7.938 -25.227 30.769 1.0 ATOM 2167 N PRO B 336 -7.937 -24.194 29.884 1.0 ATOM 2167 C PRO B 336 -7.938 -25.227 30.769 1.0 ATOM 2167 C PRO B 336 -7.938 -25.227 30.769 1.0 ATOM 2167 C PRO B 336 -7.938 -25.227 30.769 1.0 ATOM 2167 C PRO B 336 -7.938 -25.227 30.769 1.0 ATOM 2167 C PRO B 336 -7.938 -25.227 30.769 1.0 ATOM 2177 CB PRO B 336 -7.938 -25.227 3	
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ATOM 2177 CG PHE B 337 -7.229 -19.517 27.846 1.0 50 ATOM 2178 CD1 PHE B 337 -5.846 -19.511 22.002 1.0 ATOM 2179 CD2 PHE B 337 -8.023 -19.062 28.893 1.0 ATOM 2180 CE1 PHE B 337 -5.262 -19.059 29.185 1.0 ATOM 2181 CE2 PHE B 337 -7.449 -18.608 30.079 1.0 ATOM 2182 CZ PHE B 337 -6.064 -18.607 30.224 1.0	
50 ATOM 2178 CD1 PHE B 337 -5.846 -19.511 28.002 1.0 ATOM 2179 CD2 PHE B 337 -8.023 -19.062 28.893 1.0 ATOM 2180 CE1 PHE B 337 -5.262 -19.059 29.185 1.0 ATOM 2181 CE2 PHE B 337 -7.449 -18.608 30.079 1.0 ATOM 2182 CZ PHE B 337 -6.064 -18.607 30.224 1.0	
ATOM 2179 CD2 PHE B 337 -8.023 -19.062 28.893 1.0 ATOM 2180 CE1 PHE B 337 -5.262 -19.059 29.185 1.0 ATOM 2181 CE2 PHE B 337 -7.449 -18.608 30.079 1.0 ATOM 2182 CZ PHE B 337 -6.064 -18.607 30.224 1.0	
ATOM 2180 CE1 PHE B 337 -5.262 -19.059 29.185 1.6 ATOM 2181 CE2 PHE B 337 -7.449 -18.608 30.079 1.6 ATOM 2182 CZ PHE B 337 -6.064 -18.607 30.224 1.0	
ATOM 2181 CB2 PHE B 337 -7.449 -18.608 30.079 1.0 ATOM 2182 CZ PHE B 337 -6.064 -18.607 30.224 1.0	
ATOM 2182 CZ PHE B 337 -6.064 -18.607 30.224 1.0	
55 ATOM 2183 C PHE B 337 -9.420 -21.535 25.402 1.0	
ATOM 2184 O PHE B 337 -8.962 -22.399 24.658 1.0	
ATOM 2185 N SER B 338 -10.504 -20.828 25.107 1.0	
ATOM 2186 CA SER B 338 -11.198 -20.981 23.836 1.0	
ATOM 2187 CB SER B 338 -12.713 -20.948 24.035 1.0	
60 ATOM 2188 OG SER B 338 -13.164 -19.621 24.235 1.0	
ATOM 2189 C SER B 338 -10.761 -19.761 23.037 1.	
ATOM 2190 O SER B 338 -10.143 -18.855 23.591 1.0	00 34.32

	5	ATOM	2191	N	GLU	В	339	-11.075 -19.722 21.750 1.00 33.01
		ATOM	2192	CA	GLU	В	339	-10.682 -18.579 20.950 1.00 33.94
		ATOM	2193	CB	GLU	В	339	-11.146 -18.737 19.501 1.00 33.79
		ATOM	2194	CG	GLU	В	339	-10.758 -17.553 18.623 1.00 39.11
		ATOM	2195	CD	GLU	В	339	-10.865 -17.852 17.137 1.00 43.17
	10	ATOM	2196	OE1	GLU	В	339	-11.990 -17.785 16.600 1.00 45.28
	10	ATOM	2197	OE2	GLU	В	339	-9.824 -18.152 16.510 1.00 39.19
							339	-11.265 -17.295 21.531 1.00 34.28
		ATOM	2198	C	GLU	В		-10.575 -16.283 21.631 1.00 33.65
		ATOM	2199	0	GLU	В	339	
		ATOM	2200	N	ALA	В	340	-12.535 -17.339 21.920 1.00 31.12
	15	ATOM	2201	CA	ALA	В	340	-13.194 -16.164 22.469 1.00 29.10
		ATOM	2202	CB	ALA	В	340	-14.696 -16.412 22.573 1.00 33.84
		ATOM	2203	C	ALA	В	340	-12.639 -15.731 23.826 1.00 28.98
		ATOM	2204	0	ALA	В	340	-12.431 -14.541 24.060 1.00 30.48
		ATOM	2205	N	SER	В	341	-12.407 -16.691 24.719 1.00 26.66
- 1	20	ATOM	2206	CA	SER	В	341	-11.882 -16.386 26.044 1.00 24.26
		ATOM	2207	CB	SER	В	341	-11.867 -17.643 26.923 1.00 27.04
		ATOM	2208	OG	SER	В	341	-10.851 -18.541 26.515 1.00 33.84
		ATOM	2209	C	SER	В	341	-10.479 -15.793 25.960 1.00 23.97
		ATOM	2210	o	SER	В	341	-10.171 -14.824 26.651 1.00 21.56
	25	ATOM	2211	N	MET	В	342	-9.631 -16.368 25.114 1.00 26.83
5125	23	ATOM	2212	CA	MET	В	342	-8.271 -15.865 24.954 1.00 27.24
10			2212	CB	MET	В	342	-7.477 -16.758 24.001 1.00 30.45
IU		ATOM					342	-6.038 -16.300 23.802 1.00 35.35
1.0		ATOM	2214	CG	MET	В		
fut.		ATOM	2215	SD	MET	В	342	
14	30	ATOM	2216	CE	MET	В	342	-4.034 -17.341 22.244 1.00 41.37
Section .		ATOM	2217	C	MET	В	342	-8.322 -14.448 24.385 1.00 25.31
4:5		ATOM	2218	0	MET	В	342	-7.653 -13.541 24.874 1.00 26.67
9		MOTA	2219	N	MET	В	343	-9.114 -14.278 23.345 1.00 25.75
4220		ATOM	2220	CA	MET	В	343	-9.262 -12.979 22.712 1.00 25.47
La	35	ATOM	2221	CB	MET	В	343	-10.210 -13.088 21.528 1.00 23.51
W		ATOM	2222	CG	MET	В	343	-9.540 -13.618 20.273 1.00 28.86
Series Series		ATOM	2223	SD	MET	В	343	-8.325 -12.456 19.609 1.00 29.25
La la		ATOM	2224	CE	MET	В	343	-9.344 -11.015 19.371 1.00 28.74
4D		ATOM	2225	C	MET	В	343	-9.798 -11.966 23.712 1.00 25.37
D.	40	ATOM	2226	0	MET	В	343	-9.360 -10.810 23.728 1.00 24.98
		ATOM	2227	Ñ	GLY	В	344	-10.739 -12.403 24.536 1.00 23.91
		ATOM	2228	CA	GLY	В	344	-11.320 -11.526 25.536 1.00 22.43
		ATOM	2229	C	GLY	в	344	-10.313 -11.103 26.592 1.00 22.06
		ATOM	2230	Ö	GLY	В	344	-10.262 -9.934 26.982 1.00 20.87
	45	ATOM	2231	N	LEU	В	345	-9.511 -12.048 27.063 1.00 19.36
	75	ATOM	2232	CA	LEU	В	345	-8.520 -11.748 28.083 1.00 25.74
		ATOM	2233	CB	LEU	В	345	-7.886 -13.040 28.600 1.00 26.78
				CG	LEU	В	345	-8.794 -14.010 29.362 1.00 30.04
		ATOM	2234					-8.099 -15.357 29.488 1.00 28.39
		ATOM	2235	CD1	LEU	В	345	
	50	ATOM	2236	CD2	LEU	В	345	
		ATOM	2237	C	LEU	В	345	-7.425 -10.822 27.550 1.00 23.24
		ATOM	2238	0	LEU	В	345	-7.037 -9.865 28.212 1.00 23.43
		MOTA	2239	N	LEU	В	346	-6.937 -11.108 26.350 1.00 21.92
		ATOM	2240	CA	LEU	В	346	-5.874 -10.303 25.763 1.00 22.71
	55	ATOM	2241	CB	LEU	В	346	-5.343 -10.962 24.486 1.00 23.17
		ATOM	2242	CG	LEU	В	346	-4.684 -12.331 24.668 1.00 20.66
		ATOM	2243	CD1	LEU	В	346	-4.303 -12.916 23.309 1.00 18.75
		ATOM	2244	CD2	LEU	В	346	-3.464 -12.188 25.553 1.00 20.84
		ATOM	2245	C	LEU	В	346	-6.304 -8.873 25.458 1.00 22.99
	60	ATOM	2246	ō	LEU	В	346	-5.540 -7.935 25.695 1.00 22.07
		ATOM	2247	N	THR	В	347	-7.516 -8.699 24.937 1.00 20.53
		ATOM	2247	CA	THR	В	347	-7.987 -7.357 24.608 1.00 21.89
						-		

	5	ATOM	2249	CB	THR	В	347	-9.152	-7.388 23.601	1.00	21.65
	-	ATOM	2250	OG1	THR	В	347	-10.218	-8.190 24.123	1.00	19.65
		ATOM	2251	CG2	THR	В	347	-8.676	-7.955 22.262	1.00	22.01
		ATOM	2252	C	THR	В	347	-8.426	-6.590 25.853	1.00	23.60
		ATOM	2253	ō	THR	В	347	-8.358	-5.357 25.883	1.00	20.31
	10	ATOM	2254	N	ASN	В	348	-8.884	-7.314 26.874	1.00	22.27
	10	ATOM	2255	CA	ASN	В	348	-9.293	-6.667 28.114	1.00	23.99
		ATOM	2256	CB	ASN	В	348	-10.008	-7.642 29.056	1.00	22.32
		ATOM	2257	CG	ASN	В	348	-10.342	-7.022 30.398	1.00	28.26
		ATOM	2258	OD1	ASN	В	348	-9.478	-6.746 31.216	1.00	27.14
	15	ATOM	2259	ND2	ASN	В	348	-11.647	-6.764 30.625	1.00	27.02
	15	ATOM	2260	C	ASN	В	348	-8.035	-6.120 28.798	1.00	19.48
		ATOM	2261	0	ASN	В	348	-8.014	-4.991 29.271	1.00	18.26
		ATOM	2262	N	LEU	В	349	-6.984	-6.931 28.832	1.00	19.07
		ATOM	2263	CA	LEU	В	349	-5.724	-6.516 29.446	1.00	20.37
	20	ATOM	2264	CB	LEU	В	349	-4.716	-7.674 29.434	1.00	18.21
	20	ATOM	2265	CG	LEU	В	349	-3.297	-7.316 29.889	1.00	18.24
		ATOM	2266	CD1	LEU	В	349	-3.323	-6.904 31.356	1.00	12.44
		ATOM	2267	CD1	LEU	В	349	-2.370	-8.504 29.672	1.00	21.28
			2268	CD2	LEU	В	349	-5.131	-5.307 28.718	1.00	19.92
	25	ATOM	2269	0	LEU	В	349	-4.738	-4.322 29.349	1.00	16.56
155	23	ATOM ATOM	2270	N	ALA	В	350	-5.067	-5.391 27.391	1.00	16.67
123		ATOM	2270	CA	ALA	В	350	-4.529	-4.308 26.578	1.00	17.11
10		ATOM	2271	CB	ALA	В	350	-4.587	-4.690 25.095	1.00	14.15
(2)			2272	C	ALA	В	350	-5.272	-2.988 26.805	1.00	17.92
i die	30	ATOM	2274	0	ALA	В	350	-4.650	-1.926 26.904	1.00	18.71
· ·	30	ATOM	2274	N	ASP	В	351	-6.600	-3.053 26.857	1.00	17.51
312		ATOM		CA	ASP	В	351	-7.409	-1.856 27.074	1.00	16.57
1.		ATOM	2276	CB	ASP	В	351	-8.902	-2.202 27.041	1.00	18.97
.0		ATOM	2277 2278	CG	ASP	В	351	-9.785	-0.974 26.858	1.00	21.80
5 vod	35	ATOM		OD1	ASP	В	351	-9.660	-0.292 25.824	1.00	24.62
121	33	ATOM	2279	OD1	ASP	В	351	-10.604	-0.682 27.754	1.00	22.78
1,1,1		ATOM	2280 2281	C C	ASP	В	351	-7.064	-1.228 28.415	1.00	16.81
1000		MOTA	2281	0	ASP	В	351	-6.963	-0.009 28.534	1.00	15.75
1/1		MOTA		N	ARG	В	352	-6.894	-2.056 29.438	1.00	13.97
153	40	ATOM	2283 2284	CA	ARG	В	352	-6.552	-1.509 30.742	1.00	16.09
	40	ATOM		CB	ARG	В	352	-6.728	-2.571 31.833	1.00	15.78
		ATOM	2285 2286	CG	ARG	В	352	-8.189	-2.819 32.189	1.00	17.93
		MOTA		CD	ARG	В	352	-8.323	-3.882 33.279	1.00	19.84
		ATOM	2287	NE	ARG	В	352	-8.010	-5.222 32.785	1.00	21.36
	45	ATOM	2288	CZ	ARG	В	352	-7.187	-6.075 33.387	1.00	21.18
	43	ATOM	2289 2290	NH1	ARG	В	352	-6.579	-5.741 34.516	1.00	20.51
		ATOM ATOM	2291	NH2	ARG	В	352	-6.980	-7.275 32.864	1.00	28.51
				C	ARG	В	352	-5.123	-0.975 30.728	1.00	15.81
		MOTA	2292	0	ARG	В	352	-4.835	0.057 31.339	1.00	15.61
	50	ATOM	2293	N	GLU	В	353	-4.231	-1.665 30.019	1.00	15.45
	30	ATOM	2294 2295	CA	GLU	В	353	-2.838	-1.228 29.935	1.00	16.59
		ATOM		CB	GLU	В	353	-1.990	-2.243 29.168	1.00	14.64
		MOTA	2296	CG	GLU	В	353	-1.554	-3.456 29.973	1.00	18.23
		ATOM	2297			В	353	-0.620	-4.355 29.176	1.00	22.72
		ATOM	2298	CD OE1	GLU	В	353	-1.099	-5.078 28.275	1.00	21.94
	55	ATOM	2299					0.599	-4.324 29.442	1.00	24.41
		ATOM	2300	OE2	GLU	В	353	-2.729	0.119 29.219	1.00	15.85
		ATOM	2301	C	GLU	В	353	-1.872	0.119 29.219	1.00	13.76
		ATOM	2302	0	GLU	В	353	-1.872 -3.594	0.335 28.235	1.00	12.93
	CO	ATOM	2303	N	LEU	В	354		1.575 27.472	1.00	15.33
	60	ATOM	2304	CA	LEU	В	354 354	-3.556 -4.616	1.534 26.360	1.00	16.44
		ATOM	2305	CB	LEU	В			0.750 25.112	1.00	17.03
		MOTA	2306	CG	LEU	В	354	-4.174	V./50 Z5.IIZ	1.00	±1.03

	-				LEU	В	354	-5.373	0.509 24.189	1.00	16.70
	5	ATOM	2307	CD1					1.531 24.384	1.00	14.52
		ATOM	2308	CD2	LEU	В	354	-3.069			
		ATOM	2309	C	LEU	В	354	-3.747	2.805 28.361	1.00	12.78
		ATOM	2310	0	LEU	В	354	-3.123	3.850 28.141	1.00	14.28
		ATOM	2311	N	VAL	В	355	-4.600	2.682 29.369	1.00	12.60
	10	ATOM	2312	CA	VAL	В	355	-4.844	3.791 30.279	1.00	16.78
		ATOM	2313	CB	VAL	В	355	-5.925	3.429 31.327	1.00	16.84
		ATOM	2314	CG1	VAL	В	355	-6.070	4.561 32.344	1.00	19.88
		ATOM	2315	CG2	VAL	В	355	-7.254	3.187 30.639	1.00	19.33
		ATOM	2316	C	VAL	В	355	-3.533	4.161 30.986	1.00	19.17
	15	ATOM	2317	0	VAL	В	355	-3.158	5.328 31.049	1.00	17.30
	15			N	HIS	В	356	-2.826	3.160 31.499	1.00	19.68
		ATOM	2318				356	-1.559	3.418 32.177	1.00	20.64
		ATOM	2319	CA	HIS	В		-1.110	2.174 32.945	1.00	21.03
		ATOM	2320	CB	HIS	В	356				22.88
		ATOM	2321	CG	HIS	В	356	-2.018	1.818 34.085	1.00	
	20	ATOM	2322	CD2	HIS	В	356	-3.128	1.045 34.135	1.00	21.70
		ATOM	2323	ND1	HIS	В	356	-1.838	2.312 35.358	1.00	19.24
		ATOM	2324	CE1	HIS	В	356	-2.802	1.860 36.145	1.00	18.84
		ATOM	2325	NE2	HIS	В	356	-3.598	1.088 35.426	1.00	17.92
		ATOM	2326	C	HIS	В	356	-0.479	3.861 31.184	1.00	19.67
(3	25	ATOM	2327	0	HIS	В	356	0.424	4.614 31.547	1.00	19.61
		ATOM	2328	N	MET	В	357	-0.566	3.413 29.931	1.00	14.92
153		ATOM	2329	CA	MET	В	357	0.428	3.830 28.939	1.00	15.13
ru		ATOM	2330	CB	MET	В	357	0.239	3.099 27.604	1.00	13.94
10		ATOM	2331	CG	MET	В	357	1.149	3.631 26.476	1.00	14.71
good.	30			SD	MET	В	357	0.747	3.014 24.826	1.00	17.75
14	30	ATOM	2332	CE	MET	В	357	0.746	1.222 25.122	1.00	15.21
1-4		ATOM				В	357	0.316	5.334 28.699	1.00	14.94
12		ATOM	2334	C	MET				6.031 28.560	1.00	17.02
25		MOTA	2335	0	MET	В	357	1.319		1.00	18.01
THE.	1	ATOM	2336	N	ILE	В	358	-0.909	5.839 28.659		
1,1	35	ATOM	2337	CA	ILE	В	358	-1.122	7.263 28.423	1.00	19.77
i,i,j		ATOM	2338	CB	ILE	В	358	-2.634	7.577 28.287	1.00	23.11
		MOTA	2339	CG2	ILE	В	358	-2.879	9.080 28.450	1.00	25.00
43		ATOM	2340	CG1	ILE	В	358	-3.137	7.105 26.913	1.00	24.19
		ATOM	2341	CD1	ILE	В	358	-4.600	6.653 26.890	1.00	20.17
1	40	ATOM	2342	C	ILE	В	358	-0.501	8.100 29.550	1.00	22.93
		ATOM	2343	0	ILE	В	358	0.080	9.153 29.299	1.00	23.33
		ATOM	2344	N	ASN	В	359	-0.619	7.631 30.790	1.00	22.34
		ATOM	2345	CA	ASN	В	359	-0.029	8.341 31.924	1.00	23.24
		ATOM	2346	CB	ASN	В	359	-0.480	7.726 33.224	1.00	25.10
	45	ATOM	2347	CG	ASN	В	359	-1.831	8.171 33.649	1.00	32.65
	15	ATOM	2348	OD1	ASN	В	359	-2.421	9.069 33.042	1.00	32.98
		ATOM	2349	ND2	ASN	В	359	-2.364	7.549 34.691	1.00	33.87
					ASN	В	359	1.473	8.306 31.837	1.00	24.77
		ATOM	2350				359	2.152	9.285 32.149	1.00	24.19
		ATOM	2351		ASN	В		1.995	7.149 31.438	1.00	20.82
	50	ATOM	2352		TRP	В	360		6.965 31.310	1.00	19.29
		ATOM	2353	CA	TRP	В	360	3.439			18.59
		ATOM	2354		TRP	В	360	3.754	5.524 30.878	1.00	
		ATOM	2355	CG	TRP	В	360	5.085	5.363 30.176	1.00	18.21
		ATOM	2356	CD2	TRP	В	360	5.310	5.308 28.756	1.00	14.38
	55	ATOM	2357	CE2	TRP	В	360	6.698	5.129 28.561	1.00	13.42
		ATOM	2358	CE3	TRP	В	360	4.475	5.392 27.633	1.00	15.52
		ATOM	2359		TRP	В	360	6.306	5.221 30.762	1.00	13.34
		ATOM	2360		TRP	В	360	7.283	5.078 29.800	1.00	16.05
		ATOM	2361		TRP	В	360	7.272	5.032 27.288	1.00	16.84
	60	ATOM	2362		TRP	В	360	5.045	5.296 26.363	1.00	15.11
	00	ATOM	2363		TRP	В	360	6.431	5.115 26.202	1.00	16.12
		ATOM	2364		TRP	В	360	3.979	7.939 30.273	1.00	20.13
		AION	2304	_	TICE		500				

	5	ATOM	2365	0	TRP	В	360	4.991	8.606 30.497	1.00	17.26
		ATOM	2366	N	ALA	В	361	3.295	8.012 29.135	1.00	19.34
		ATOM	2367	CA	ALA	В	361	3.708	8.900 28.051	1.00	22.01
		ATOM	2368	CB	ALA	В	361	2.682	8.855 26.921	1.00	19.53
		ATOM	2369	C	ALA	В	361	3.883	10.336 28.552	1.00	22.39
	10	ATOM	2370	0	ALA	В	361	4.858	11.005 28.210		19.57
	10						362	2.932	10.794 29.361		21.96
		ATOM	2371	N	LYS	В			12.139 29.923		26.45
		ATOM	2372	CA	LYS	В	362	2.966			
		ATOM	2373	CB	LYS	В	362	1.741	12.363 30.811		29.79
		ATOM	2374	CG	LYS	В	362	0.426	12.417 30.064		33.57
	15	ATOM	2375	CD	LYS	В	362	-0.563	13.304 30.805		36.83
		ATOM	2376	CE	LYS	В	362	-1.620	12.490 31.512	1.00	36.89
		ATOM	2377	NZ	LYS	В	362	-2.873	13.276 31.664	1.00	39.07
		ATOM	2378	C	LYS	В	362	4.223	12.379 30.757	1.00	27.77
		ATOM	2379	0	LYS	В	362	4.661	13.517 30.922	1.00	26.93
	20	ATOM	2380	N	ARG	В	363	4.805	11.302 31.278	1.00	26.61
	20	ATOM	2381	CA	ARG	В	363	5.996	11.414 32.109		27.74
				CB	ARG	В	363	5.887	10.457 33.298		28.93
		ATOM	2382	CG	ARG	В	363	4.650	10.704 34.158		36.07
		ATOM	2383					4.569	9.745 35.344		42.83
		ATOM	2384	CD	ARG	В	363				49.79
1110	25	ATOM	2385	NE	ARG	В	363	4.477	8.344 34.928		
123		ATOM	2386	CZ	ARG	В	363	3.395	7.582 35.080		51.48
5 3.5		ATOM	2387	NH1	ARG	В	363	2.300	8.081 35.648		52.17
to		ATOM	2388	NH2	ARG	В	363	3.405	6.316 34.668		40.24
Irdi.		ATOM	2389	C	ARG	В	363	7.308	11.190 31.367		25.80
1	30	ATOM	2390	0	ARG	В	363	8.374	11.183 31.975	1.00	29.36
[nh		ATOM	2391	N	VAL	В	364	7.231	11.009 30.053	1.00	24.28
1		ATOM	2392	CA	VAL	В	364	8.431	10.823 29.248	1.00	21.87
		ATOM	2393	CB	VAL	В	364	8.116	10.048 27.947	1.00	21.84
10 1000		ATOM	2394	CG1	VAL	В	364	9.267	10.184 26.968	1.00	15.85
13	35	ATOM	2395	CG2	VAL	В	364	7.860	8.560 28.268	1.00	16.24
1,4	55	ATOM	2396	C	VAL	В	364	8.925	12.241 28.923		28.14
1,1			2390	0	VAL	В	364	8.219	13.023 28.289		24.24
(700)		ATOM				В	365	10.141	12.591 29.375		28.57
40		ATOM	2398	N	PRO			11.061	11.726 30.13		30.58
* 17.1	40	MOTA	2399	CD	PRO	В	365		13.919 29.138		32.16
145	40	ATOM	2400	CA	PRO	В	365	10.719			
		ATOM	2401	CB	PRO	В	365	12.189	13.739 29.50		32.70
		ATOM	2402	CG	PRO	В	365	12.170	12.671 30.545		33.35
		ATOM	2403	C	PRO	В	365	10.546	14.464 27.72		32.22
		ATOM	2404	0	PRO	В	365	11.056	13.897 26.76		37.04
	45	ATOM	2405	N	GLY	В	366	9.821	15.570 27.60		34.09
		ATOM	2406	CA	GLY	В	366	9.612	16.182 26.310	1.00	32.54
		ATOM	2407	C	GLY	В	366	8.241	15.969 25.700	1.00	33.46
		ATOM	2408	0	GLY	В	366	7.791	16.779 24.88	1.00	33.73
		ATOM	2409	N	PHE	В	367	7.564	14.895 26.09	1.00	31.08
	50	ATOM	2410	CA	PHE	В	367	6.250	14.593 25.54	2 1.00	28.60
	50	ATOM	2411	CB	PHE	В	367	5.745	13.244 26.05		25.96
				CG	PHE	В	367	4.629	12.671 25.23		22.75
		ATOM	2412					3.313	12.771 25.66		22.62
		ATOM	2413	CD1	PHE	В	367				22.29
		ATOM	2414	CD2	PHE	В	367	4.897	12.025 24.03		
	55	ATOM	2415	CE1	PHE	В	367	2.272	12.233 24.91		25.63
		ATOM	2416	CE2	PHE	В	367	3.867	11.486 23.27		20.82
		ATOM	2417	CZ	PHE	В	367	2.553	11.588 23.71		25.50
		ATOM	2418	C	PHE	В	367	5.178	15.646 25.78	1 1.00	26.79
		ATOM	2419	0	PHE	В	367	4.458	16.001 24.85	1.00	23.37
	60	ATOM	2420	N	VAL	В	368	5.049	16.143 27.00	9 1.00	31.26
	00	ATOM	2421	CA	VAL	В	368	4.020	17.151 27.27		35.71
		ATOM	2422	CB	VAL	В	368	3.817	17.412 28.79		35.98
		AT ON	2422	CD		_					

	5	ATOM	2423	CG1	VAL	В	368	2.944	16.320 29.392	1.00	37.64
	-	ATOM	2424	CG2	VAL	В	368	5.157	17.495 29.508	1.00	35.81
		ATOM	2425	C	VAL	В	368	4.328	18.482 26.598	1.00	35.87
		ATOM	2426	0	VAL	В	368	3.450	19.330 26.457	1.00	37.71
				N	ASP	В	369	5.572	18.665 26.175	1.00	35.49
	10	MOTA	2427					5.950	19.904 25.503	1.00	36.54
	10	ATOM	2428	CA	ASP	В	369				39.79
		ATOM	2429	CB	ASP	В	369	7.466	19.963 25.309	1.00	
		ATOM	2430	CG	ASP	В	369	8.213	20.169 26.615	1.00	44.33
		ATOM	2431	OD1	ASP	В	369	9.409	19.807 26.684	1.00	48.45
		ATOM	2432	OD2	ASP	В	369	7.604	20.693 27.572	1.00	43.27
	15	ATOM	2433	C	ASP	В	369	5.248	19.997 24.149	1.00	34.49
		ATOM	2434	0	ASP	В	369	5.131	21.074 23.571	1.00	34.51
		ATOM	2435	N	LEU	В	370	4.776	18.859 23.653	1.00	30.97
		ATOM	2436	CA	LEU	В	370	4.086	18.809 22.370	1.00	29.80
		MOTA	2437	CB	LEU	В	370	4.145	17.389 21.799	1.00	27.27
	20	ATOM	2438	CG	LEU	В	370	5.522	16.733 21.688	1.00	28.07
		ATOM	2439	CD1	LEU	В	370	5.353	15.242 21.400	1.00	30.38
		ATOM	2440	CD2	LEU	В	370	6.316	17.396 20.574	1.00	22.82
		ATOM	2441	C	LEU	В	370	2.628	19.218 22.521	1.00	28.04
				0	LEU	В	370	2.066	19.151 23.611	1.00	29.71
	25	ATOM	2442	N		В	371	2.011	19.645 21.425	1.00	28.70
(1)	23	ATOM	2443		THR	В	371	0.602	20.014 21.474	1.00	30.31
157		ATOM	2444	CA	THR				20.690 20.163	1.00	31.96
10		MOTA	2445	CB	THR	В	371	0.150			29.49
10		ATOM	2446	OG1	THR	В	371	0.284	19.763 19.080	1.00	
- Beatle		ATOM	2447	CG2	THR	В	371	0.991	21.930 19.878	1.00	29.98
112	30	MOTA	2448	C	THR	В	371	-0.208	18.726 21.666	1.00	30.59
115		MOTA	2449	0	THR	В	371	0.300	17.624 21.431	1.00	27.10
14		ATOM	2450	N	LEU	В	372	-1.461	18.863 22.087	1.00	27.65
n		MOTA	2451	CA	LEU	В	372	-2.323	17.702 22.303	1.00	30.86
1,3		ATOM	2452	CB	LEU	В	372	-3.722	18.147 22.737	1.00	30.11
1,4	35	ATOM	2453	CG	LEU	В	372	-4.715	17.006 22.960	1.00	32.80
LU		ATOM	2454	CD1	LEU	В	372	-4.231	16.147 24.126	1.00	34.10
1,63		MOTA	2455	CD2	LEU	В	372	-6.105	17.562 23.246	1.00	31.16
100		ATOM	2456	C	LEU	В	372	-2.437	16.863 21.034	1.00	31.77
10		ATOM	2457	0	LEU	В	372	-2.417	15.629 21.078	1.00	27.06
40	40	ATOM	2458	N	HIS	В	373	-2.564	17.548 19.905	1.00	31.30
		ATOM	2459	CA	HIS	В	373	-2.685	16.888 18.614	1.00	31.35
		MOTA	2460	CB	HIS	В	373	-2.844	17.935 17.503	1.00	34.30
		ATOM	2461	CG	HIS	В	373	-2.503	17.430 16.132	1.00	41.27
		ATOM	2462	CD2	HIS	В	373	-3.293	17.105 15.079	1.00	42.50
	45		2463	ND1	HIS	В	373	-1.205	17.220 15.715	1.00	43.69
	43	ATOM					373	-1.210	16.787 14.465	1.00	48.87
		MOTA	2464	CE1	HIS	В		-2.465	16.708 14.056	1.00	43.72
		ATOM	2465	NE2	HIS	В	373			1.00	28.29
		ATOM	2466	С	HIS	В	373	-1.468	16.012 18.337		
		MOTA	2467	0	HIS	В	373	-1.610	14.878 17.897	1.00	30.21
	50	ATOM	2468	N	ASP	В	374	-0.275	16.541 18.589	1.00	28.85
		MOTA	2469	CA	ASP	В	374	0.950	15.783 18.350	1.00	28.28
		MOTA	2470	CB	ASP	В	374	2.178	16.678 18.535	1.00	31.33
		ATOM	2471	CG	ASP	В	374	2.433	17.577 17.333	1.00	39.07
		ATOM	2472	OD1	ASP	В	374	3.195	18.557 17.478	1.00	40.60
	55	ATOM	2473	OD2	ASP	В	374	1.874	17.305 16.246	1.00	38.64
		ATOM	2474	C	ASP	В	374	1.029	14.592 19.303	1.00	29.05
		ATOM	2475	ō	ASP	В	374	1.432	13.494 18.908	1.00	24.26
		MOTA	2476	N	GLN	В	375	0.642	14.814 20.556	1.00	24.52
		ATOM	2477	CA	GLN	В	375	0.667	13.749 21.547	1.00	27.37
	60	ATOM	2478	CB	GLN	В	375	0.213	14.270 22.901	1.00	26.66
	~~	ATOM	2479	CG	GLN	В	375	1.164	15.236 23.563	1.00	29.74
		ATOM	2480	CD	GLN	В	375	0.623	15.691 24.890	1.00	33.13
		ALOM	2-30	CD	0224	_	5.5	102		-	-

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	5	ATOM	2481	OE1	GLN	В	375	-0.044			
		ATOM	2482	NE2	GLN	В	375	0.895	16.953 25.236	1.00	33.98
		ATOM	2483	C	GLN	В	375	-0.259	12.630 21.104	1.00	24.52
		ATOM	2484	0	GLN	В	375	0.074	11.451 21.221	1.00	23.56
		ATOM	2485	N	VAL	В	376	-1.426	13.013 20.599	1.00	21.87
	10	ATOM	2486	CA	VAL	В	376	-2.409	12.055 20.140	1.00	23.44
	10										
		MOTA	2487	CB	VAL	В	376	-3.718	12.760 19.717	1.00	22.09
		ATOM	2488	CG1	VAL	В	376	-4.572	11.823 18.877	1.00	24.14
		ATOM	2489	CG2	VAL	В	376	-4.486	13.192 20.954	1.00	16.96
		ATOM	2490	C	VAL	В	376	-1.852	11.257 18.965	1.00	24.15
	15	ATOM	2491	0	VAL	В	376	-1.949	10.032 18.938	1.00	22.26
		ATOM	2492	N	HIS	В	377	-1.251	11.953 18.007	1.00	25.85
			2493	CA	HIS	В	377	-0.689	11.284 16.843	1.00	25.68
		ATOM									25.27
		ATOM	2494	CB	HIS	В	377	-0.078	12.306 15.886	1.00	
		ATOM	2495	CG	HIS	В	377	0.535	11.690 14.667	1.00	30.63
	20	MOTA	2496	CD2	HIS	В	377	1.828	11.559 14.287	1.00	31.03
		ATOM	2497	ND1	HIS	В	377	-0.217	11.086 13.683	1.00	35.05
		ATOM	2498	CE1	HIS	В	377	0.588	10.607 12.750	1.00	33.12
		ATOM	2499	NE2	HIS	В	377	1.833	10.882 13.093	1.00	31.06
		ATOM	2500	C	HIS	В	377	0.365	10.237 17.210	1.00	24.37
	25						377	0.321	9.109 16.719	1.00	21.47
	1947	ATOM	2501	0	HIS	В					19.24
4	2	ATOM	2502	N	LEU	В	378	1.307	10.609 18.072	1.00	
1	13	ATOM	2503	CA	LEU	В	378	2.365	9.691 18.474	1.00	20.09
1	Ø	ATOM	2504	CB	LEU	В	378	3.363	10.402 19.388	1.00	18.64
	rafe	ATOM	2505	CG	LEU	В	378	4.230	11.489 18.736	1.00	22.15
	30	ATOM	2506	CD1	LEU	В	378	5.104	12.148 19.796	1.00	22.51
	-	ATOM	2507	CD2	LEU	В	378	5.094	10.885 17.638	1.00	20.68
	nds.	ATOM	2508	C	LEU	В	378	1.832	8.433 19.161	1.00	18.91
	ni.			0	LEU	В	378	2.262	7.320 18.859	1.00	17.52
		MOTA	2509								18.25
4	35	MOTA	2510	N	LEU	В	379	0.888	8.610 20.077	1.00	
1	35	MOTA	2511	CA	LEU	В	379	0.317	7.486 20.795	1.00	18.60
5	.5	ATOM	2512	CB	LEU	В	379	-0.526	7.989 21.968	1.00	16.77
24	J.	ATOM	2513	CG	LEU	В	379	0.292	8.353 23.214	1.00	17.90
1	isoli iso	ATOM	2514	CD1	LEU	В	379	-0.578	9.092 24.211	1.00	15.84
	J	ATOM	2515	CD2	LEU	В	379	0.851	7.075 23.842	1.00	22.09
à,	40	ATOM	2516	C	LEU	В	379	-0.518	6.605 19.872	1.00	20.17
	40			0	LEU	В	379	-0.476	5.377 19.968	1.00	18.11
		ATOM	2517						7.222 18.971	1.00	19.40
		MOTA	2518	N	GLU	В	380	-1.273			
		MOTA	2519	CA	GLU	В	380	-2.086	6.435 18.049	1.00	20.19
		ATOM	2520	CB	GLU	В	380	-2.994	7.350 17.222	1.00	22.43
	45	ATOM	2521	CG	GLU	В	380	-4.182	7.874 18.007	1.00	25.30
		ATOM	2522	CD	GLU	В	380	-5.070	8.789 17.188	1.00	29.44
		ATOM	2523	OE1	GLU	В	380	-6.206	9.066 17.625	1.00	31.70
		ATOM	2524	OE2	GLU	В	380	-4.631	9.230 16.110	1.00	31.75
			2525	C	GLU	В	380	-1.210	5.594 17.117	1.00	18.92
	CO	ATOM							4.491 16.722	1.00	19.83
	50	ATOM	2526	0	GLU	В	380	-1.586			
		ATOM	2527	N	ACYS	В	381	-0.039	6.113 16.772	0.75	17.41
		ATOM	2528	N	BCYS	В	381	-0.035	6.113 16.779	0.25	17.76
		MOTA	2529	CA	ACYS	В	381	0.860	5.384 15.887	0.75	20.19
		ATOM	2530	CA	BCYS	В	381	0.875	5.407 15.884	0.25	17.50
	55	ATOM	2531	CB	ACYS	В	381	1.870	6.342 15.248	0.75	24.20
	55	ATOM	2532	CB	BCYS	В	381	1.830	6.406 15.226	0.25	16.63
				SG	ACYS	В	381	1.167	7.518 14.060	0.75	33.54
		ATOM	2533			_				0.75	10.36
		MOTA	2534	SG	BCYS	В	381	3.048	5.656 14.128		
		ATOM	2535	C	ACYS	В	381	1.626	4.269 16.592	0.75	20.59
	60	ATOM	2536	C	BCYS	В	381	1.689	4.305 16.561	0.25	19.19
		ATOM	2537	0	ACYS	В	381	1.737	3.161 16.069	0.75	19.16
		ATOM	2538	0	BCYS	В	381	1.904	3.241 15.982	0.25	19.25

	5	ATOM	2539	N	ALA	В	382	2.134	4.560 17.785	1.00	19.04
		ATOM	2540	CA	ALA	В	382	2.955	3.602 18.530	1.00	20.27
		ATOM	2541	CB	ALA	В	382	4.135	4.364 19.143	1.00	18.68
		ATOM	2542	C	ALA	В	382	2.356	2.702 19.607	1.00	16.82
		ATOM	2543	0	ALA	В	382	3.070	1.852 20.142	1.00	13.37
	10	ATOM	2544	N	TRP	В	383	1.074	2.855 19.916	1.00	15.30
		ATOM	2545	CA	TRP	В	383	0.487	2.089 21.013	1.00	15.80
		ATOM	2546	CB	TRP	В	383	-1.009	2.410 21.160	1.00	16.63
		ATOM	2547	CG	TRP	В	383	-1.871	1.775 20.129	1.00	19.93
		ATOM	2548	CD2	TRP	В	383	-2.493	0.483 20.198	1.00	20.80
	15	ATOM	2549	CE2	TRP	В	383	-3.226	0.309 19.003	1.00	19.27
		ATOM	2550	CE3	TRP	В	383	-2.506	-0.542 21.155	1.00	21.32
		ATOM	2551	CD1	TRP	В	383	-2.236	2.312 18.933	1.00	18.59
		ATOM	2552	NE1	TRP	В	383	-3.051	1.439 18.250	1.00	23.67
		ATOM	2553	CZ2	TRP	В	383	-3.963	-0.853 18.733	1.00	21.55
	20	ATOM	2554	CZ3	TRP	В	383	-3.243	-1.702 20.888	1.00	20.29
	20	ATOM	2555	CH2	TRP	В	383	-3.960	-1.844 19.686	1.00	19.03
		ATOM	2556	C	TRP	В	383	0.701	0.579 21.020	1.00	17.35
			2557	0	TRP	В	383	0.982	0.010 22.077	1.00	13.92
		ATOM	2558	N	LEU	В	384	0.568	-0.087 19.879	1.00	14.07
	25	MOTA			LEU	В	384	0.773	-1.532 19.903	1.00	15.98
1	23	MOTA	2559	CA			384	0.181	-2.200 18.656	1.00	12.19
411		MOTA	2560	CB	LEU	В		0.173	-3.735 18.720	1.00	12.13
T		ATOM	2561	CG	LEU	В	384		-4.240 20.089	1.00	10.65
00		ATOM	2562	CD1	LEU	В	384	-0.352	-4.259 17.586	1.00	17.84
luk:	20	ATOM	2563	CD2	LEU	В	384	-0.707			14.64
14	30	ATOM	2564	C	LEU	В	384	2.262	-1.861 20.034	1.00	
144		ATOM	2565	0	LEU	В	384	2.627	-2.833 20.690	1.00	13.78
1200		ATOM	2566	N	GLU	В	385	3.116	-1.046 19.414	1.00	14.96
87		ATOM	2567	CA	GLU	В	385	4.565	-1.260 19.509	1.00	13.79
13		ATOM	2568	CB	GLU	В	385	5.336	-0.179 18.739	1.00	15.34
L.J	35	ATOM	2569	CG	GLU	В	385	5.297	-0.312 17.207	1.00	15.38
W		ATOM	2570	CD	GLU	В	385	6.162	0.738 16.520	1.00	23.97
		ATOM	2571	OE1	GLU	В	385	7.381	0.500 16.358	1.00	21.03
10		ATOM	2572	OE2	GLU	В	385	5.622	1.808 16.149	1.00	22.19
10		MOTA	2573	C	GLU	В	385	4.963	-1.161 20.987	1.00	15.79
182	40	ATOM	2574	0	GLU	В	385	5.788	-1.942 21.463	1.00	15.04
		MOTA	2575	N	ILE	В	386	4.389	-0.213 21.690	1.00	13.32
		MOTA	2576	CA	ILE	В	386	4.723	-0.019 23.108	1.00	14.06
		ATOM	2577	CB	ILE	В	386	4.173	1.326 23.614	1.00	15.36
		ATOM	2578	CG2	ILE	В	386	4.374	1.451 25.130	1.00	15.97
	45	ATOM	2579	CG1	ILE	В	386	4.910	2.476 22.907	1.00	17.95
		ATOM	2580	CD1	ILE	В	386	4.118	3.768 22.874	1.00	21.12
		ATOM	2581	C	ILE	В	386	4.227	-1.164 23.993	1.00	14.97
		ATOM	2582	0	ILE	В	386	4.905	-1.560 24.941	1.00	19.60
		ATOM	2583	N	LEU	В	387	3.038	-1.675 23.709	1.00	15.18
	50	ATOM	2584	CA	LEU	В	387	2.516	-2.791 24.478	1.00	15.98
		ATOM	2585	CB	LEU	В	387	1.070	-3.097 24.080	1.00	17.15
		ATOM	2586	CG	LEU	В	387	-0.031	-2.113 24.486	1.00	19.65
		ATOM	2587	CD1	LEU	В	387	-1.371	-2.628 23.972	1.00	17.77
		ATOM	2588	CD2	LEU	В	387	-0.075	-1.966 26.002	1.00	15.38
	55	ATOM	2589	C	LEU	В	387	3.391	-4.013 24.180	1.00	14.69
	22	ATOM	2590	ō	LEU	В	387	3.712	-4.792 25.076	1.00	14.03
		ATOM	2591	N	MET	В	388	3.785	-4.178 22.921	1.00	16.43
		ATOM	2592	CA	MET	В	388	4.602	-5.329 22.547	1.00	16.67
		ATOM	2593	CB	MET	В	388	4.673	-5.460 21.026	1.00	14.83
	60	ATOM	2594	CG	MET	В	388	3.403	-6.066 20.453	1.00	13.91
	00		2595	SD	MET	В	388	3.364	-6.193 18.675		17.23
		MOTA	2595 2596	CE	MET	В	388	1.906	-7.225 18.511	1.00	14.97
		ATOM	∠596	CE.	PEL		200	1.500	7.223 10.311	1.00	

	5	ATOM	2597	C	MET	В	388	6.004	-5.332	23.133	1.00	20.19
		ATOM	2598	0	MET	В	388	6.460	-6.366	23.636	1.00	21.50
		ATOM	2599	N	ILE	В	389	6.707	-4.203	23.074	1.00	15.34
		ATOM	2600	CA	ILE	В	389	8.044	-4.209	23.634	1.00	15.59
		ATOM	2601	CB	ILE	В	389	8.836	-2.911	23.322	1.00	14.95
	10	ATOM	2602	CG2	ILE	В	389	8.330	-1.746		1.00	12.81
	10		2603	CG1	ILE	В	389	10.325	-3.164		1.00	17.24
		ATOM					389	11.228	-1.972		1.00	15.65
		ATOM	2604	CD1	ILE	В						14.30
		ATOM	2605	C	ILE	В	389	7.950	-4.446		1.00	
		ATOM	2606	0	ILE	В	389	8.844	-5.044		1.00	18.72
	15	ATOM	2607	N	GLY	В	390	6.855	-4.007		1.00	13.99
		ATOM	2608	CA	GLY	В	390	6.681	-4.219		1.00	14.87
		ATOM	2609	C	GLY	В	390	6.444	-5.702	27.463	1.00	18.54
		ATOM	2610	0	GLY	В	390	6.989	-6.282	28.403	1.00	16.54
		ATOM	2611	N	LEU	В	391	5.623	-6.325	26.628	1.00	16.15
	20	ATOM	2612	CA	LEU	В	391	5.334	-7.743	26.775	1.00	18.91
	20	ATOM	2613	CB	LEU	В	391	4.332	-8.179		1.00	19.55
		ATOM	2614	CG	LEU	В	391	4.157	-9.689		1.00	20.91
						В	391	3.580	-10.351		1.00	19.41
		MOTA	2615	CD1	LEU			3.232	-9.913		1.00	20.70
		ATOM	2616	CD2	LEU	В	391					20.70
13	25	ATOM	2617	C	LEU	В	391	6.649	-8.518		1.00	
123		ATOM	2618	0	LEU	В	391	7.002	-9.352		1.00	18.66
[1]		ATOM	2619	N	VAL	В	392	7.378	-8.215		1.00	18.71
123		ATOM	2620	CA	VAL	В	392	8.649	-8.868		1.00	19.51
ind.		ATOM	2621	CB	VAL	В	392	9.288	-8.281	24.005	1.00	23.77
74	30	ATOM	2622	CG1	VAL	В	392	10.751	-8.687	23.920	1.00	24.63
jul.		ATOM	2623	CG2	VAL	В	392	8.520	-8.773	22.767	1.00	19.94
		ATOM	2624	C	VAL	В	392	9.615	-8.707	26.450	1.00	22.80
12.5		ATOM	2625	0	VAL	В	392	10.336	-9.637	26.811	1.00	19.36
33		ATOM	2626	N	TRP	В	393	9.617	-7.522		1.00	22.10
	35	ATOM	2627	CA	TRP	В	393	10.492	-7.241	28.171	1.00	23.20
14	55	ATOM	2628	CB	TRP	В	393	10.388	-5.773		1.00	19.22
1				CG	TRP	В	393	11.056	-5.479		1.00	22.53
100		ATOM	2629			В	393	12.453	-5.591		1.00	20.36
1		ATOM	2630	CD2	TRP			12.624	-5.208		1.00	25.65
10	40	ATOM	2631	CE2	TRP	В	393		-5.976		1.00	22.12
19.50	40	ATOM	2632	CE3	TRP	В	393	13.578				
		ATOM	2633	CD1	TRP	В	393	10.452	-5.046		1.00	23.02
		MOTA	2634	NE1	TRP	В	393	11.387	-4.881		1.00	24.91
		ATOM	2635	CZ2	TRP	В	3 9 3	13.876	-5.200		1.00	23.00
		ATOM	2636	CZ3	TRP	В	393	14.829	-5.968		1.00	23.98
	45	ATOM	2637	CH2	TRP	В	3 9 3	14.964	-5.582	31.423	1.00	23.20
		ATOM	2638	C	TRP	В	3 9 3	10.208	-8.114	29.388	1.00	24.36
		ATOM	2639	0	TRP	В	393	11.128	-8.717	29.944	1.00	23.04
		ATOM	2640	N	ARG	В	394	8.952	-8.189	29.819	1.00	21.29
		ATOM	2641	CA	ARG	В	394	8.680	-9.003	30.990	1.00	22.43
	50	ATOM	2642	CB	ARG	В	394	7.365	-8.601		1.00	23.97
	50		2643	CG	ARG	В	394	6.259		30.759	1.00	26.16
		ATOM				В	394	5.026		31.574	1.00	20.86
		ATOM	2644	CD	ARG					30.786	1.00	19.54
		ATOM	2645	NE	ARG	В	394	3.817				
		ATOM	2646	CZ	ARG	В	394	3.327		29.915	1.00	20.58
	55	ATOM	2647	NH1	ARG	В	394	3.944		29.722	1.00	17.41
		ATOM	2648	NH2	ARG	В	394	2.229		29.220	1.00	16.82
		ATOM	2649	C	ARG	В	394	8.695	-10.502		1.00	21.78
		ATOM	2650	0	ARG	В	394	8.657	-11.294	31.648	1.00	23.44
		ATOM	2651	N	SER	В	395	8.767	-10.880	29.438	1.00	17.10
	60	ATOM	2652	CA	SER	В	395	8.805	-12.289	29.041	1.00	25.08
	-	ATOM	2653	CB	SER	В	395	8.206	-12.473		1.00	19.47
		ATOM	2654	OG	SER	В	395	6.832	-12.136		1.00	21.73
		MI ON	2034	00	C Land		223					

	_			~	a mp		205	10.239 -12.831 29.031 1.00 26.29
	5	MOTA	2655	C	SER	В	395	
		ATOM	2656	0	SER	В	395	10.458 -14.030 28.854 1.00 23.75
		ATOM	2657	N	MET	В	396	11.206 -11.938 29.210 1.00 30.79
		ATOM	2658	CA	MET	В	396	12.620 -12.307 29.205 1.00 35.07
		ATOM	2659	CB	MET	В	396	13.479 -11.063 29.423 1.00 33.84
	10	ATOM	2660	CG	MET	В	396	14.155 -10.569 28.171 1.00 36.88
	10	ATOM	2661	SD	MET	В	396	15.149 -9.127 28.491 1.00 40.96
		MOTA	2662	CE	MET	В	396	
		ATOM	2663	C	MET	В	396	12.983 -13.353 30.250 1.00 35.88
		ATOM	2664	0	MET	В	396	13.828 -14.215 30.011 1.00 34.52
	15	ATOM	2665	N	GLU	В	397	12.348 -13.266 31.410 1.00 36.19
		ATOM	2666	CA	GLU	В	397	12.604 -14.206 32.492 1.00 39.24
		ATOM	2667	CB	GLU	В	397	12.153 -13.605 33.821 1.00 44.38
		ATOM	2668	CG	GLU	В	397	12.983 -12.422 34.271 1.00 54.05
					GLU	В	397	13.483 -12.587 35.686 1.00 56.78
	20	ATOM	2669	CD				13.380 -11.621 36.470 1.00 60.90
	20	ATOM	2670	OE1	GLU	В	397	
		ATOM	2671	OE2	GLU	В	397	13.975 -13.688 36.013 1.00 60.82
		ATOM	2672	C	GLU	В	397	11.878 -15.528 32.273 1.00 36.65
		ATOM	2673	0	GLU	В	397	12.021 -16.459 33.061 1.00 35.84
		ATOM	2674	N	HIS	В	398	11.100 -15.609 31.202 1.00 32.14
1225	25	ATOM	2675	CA	HIS	В	398	10.347 -16.823 30.914 1.00 29.48
123	20	ATOM	2676	CB	HIS	В	398	8.863 -16.567 31.178 1.00 29.87
1					HIS	В	398	8.582 -16.111 32.574 1.00 31.80
ii.		ATOM	2677	CG				
(13)		MOTA	2678	CD2	HIS	В	398	
lain.		MOTA	2679	ND1	HIS	В	398	8.727 -14.799 32.972 1.00 33.27
4	30	ATOM	2680	CE1	HIS	В	398	8.462 -14.701 34.262 1.00 32.19
jub.		ATOM	2681	NE2	HIS	В	398	8.148 -15.902 34.714 1.00 33.48
1		ATOM	2682	C	HIS	В	398	10.556 -17.317 29.492 1.00 25.95
		ATOM	2683	0	HIS	В	398	9.637 -17.291 28.672 1.00 27.47
51		ATOM	2684	N	PRO	В	399	11.771 -17.801 29.186 1.00 29.09
1111	35		2685	CD	PRO	В	399	12.926 -17.922 30.096 1.00 29.93
i,U	33	ATOM						12.079 -18.300 27.845 1.00 27.40
1.1		MOTA	2686	CA	PRO	В	399	
1.5		MOTA	2687	CB	PRO	В	399	
ŧŪ.		MOTA	2688	CG	PRO	В	399	14.062 -18.284 29.170 1.00 30.81
111		MOTA	2689	C	PRO	В	399	11.009 -19.246 27.319 1.00 29.76
122	40	ATOM	2690	0	PRO	В	399	10.552 -20.137 28.035 1.00 29.18
		ATOM	2691	N	GLY	В	400	10.601 -19.035 26.071 1.00 27.45
		ATOM	2692	CA	GLY	В	400	9.588 -19.884 25.466 1.00 26.93
		ATOM	2693	C	GLY	В	400	8.161 -19.537 25.849 1.00 26.73
			2694	o	GLY	В	400	7.220 -20.153 25.356 1.00 28.36
	15	ATOM					401	7.996 -18.554 26.727 1.00 25.50
	45	ATOM	2695	N	LYS	В		
		ATOM	2696	CA	LYS	В	401	
		ATOM	2697	CB	LYS	В	401	6.435 -18.563 28.619 1.00 28.50
		ATOM	2698	CG	LYS	В	401	6.476 -20.069 28.879 1.00 28.58
		ATOM	2699	CD	LYS	В	401	6.181 -20.353 30.349 1.00 35.47
	50	ATOM	2700	CE	LYS	В	401	6.073 -21.847 30.635 1.00 38.59
	-	ATOM	2701	NZ	LYS	В	401	7.177 -22.611 29.989 1.00 42.39
			2702	C	LYS	В	401	6.493 -16.622 27.060 1.00 21.78
		ATOM					401	7.465 -15.872 27.035 1.00 21.45
		ATOM	2703	0	LYS	В		
		ATOM	2704	N	LEU	В	402	•
	55	ATOM	2705	CA	LEU	В	402	4.929 -14.759 26.925 1.00 21.37
		ATOM	2706	CB	LEU	В	402	4.088 -14.449 25.689 1.00 18.47
		ATOM	2707	CG	LEU	В	402	4.798 -14.673 24.360 1.00 16.89
		ATOM	2708	CD1	LEU	В	402	3.821 -14.395 23.211 1.00 21.23
		ATOM	2709	CD2	LEU	В	402	6.011 -13.760 24.277 1.00 23.15
	60	ATOM	2710	C	LEU	В	402	4.147 -14.399 28.179 1.00 19.66
	00			0	LEU	В	402	3.024 -14.880 28.381 1.00 18.05
		ATOM	2711					4.743 -13.559 29.019 1.00 19.54
		ATOM	2712	N	LEU	В	403	4.743 -13.337 27.017 1.00 19.34

	5	ATOM	2713	CA	LEU	В	403	4.099 -13.148 30.259 1.00 20.21
		ATOM	2714	CB	LEU	В	403	5.155 -12.856 31.332 1.00 23.16
		ATOM	2715	CG	LEU	В	403	4.639 -12.682 32.766 1.00 29.54
		ATOM	2716	CD1	LEU	В	403	5.519 -13.450 33.728 1.00 32.67
		ATOM	2717	CD2	LEU	В	403	4.626 -11.213 33.138 1.00 32.38
	10	ATOM	2718	C	LEU	В	403	3.219 -11.918 30.043 1.00 20.42
	10	ATOM	2719	0	LEU	В	403	3.638 -10.787 30.291 1.00 19.18
		ATOM	2720	N	PHE	В	404	2.003 -12.145 29.565 1.00 21.44
		ATOM	2721	CA	PHE	В	404	1.066 -11.053 29.340 1.00 21.69
		ATOM	2722	CB	PHE	В	404	-0.199 -11.598 28.687 1.00 17.26
	15		2723	CG	PHE	В	404	-0.026 -11.897 27.227 1.00 19.75
	13	ATOM ATOM	2724	CD1	PHE	В	404	0.364 -13.167 26.801 1.00 17.90
			2724	CD2	PHE	В	404	-0.210 -10.897 26.280 1.00 17.04
		ATOM ATOM	2726	CE1	PHE	В	404	0.572 -13.434 25.447 1.00 19.88
		ATOM	2727	CE2	PHE	В	404	-0.007 -11.148 24.924 1.00 18.47
	20		2728	CZ	PHE	В	404	0.386 -12.418 24.503 1.00 16.45
	20	ATOM ATOM	2729	C	PHE	В	404	0.768 -10.403 30.685 1.00 21.95
				0	PHE	В	404	0.656 -9.177 30.804 1.00 22.99
		MOTA	2730	N	ALA	В	405	0.670 -11.247 31.702 1.00 21.12
		MOTA	2731	CA	ALA	В	405	0.424 -10.814 33.066 1.00 22.43
	25	MOTA	2732			В		-1.074 -10.603 33.304 1.00 24.69
1	25	ATOM	2733	CB	ALA ALA	В	405 405	0.959 -11.926 33.962 1.00 22.40
à É)	MOTA	2734	C		В	405	1.133 -13.061 33.517 1.00 21.67
210	1	ATOM	2735	O N	ALA PRO	В	405	1.246 -11.612 35.230 1.00 25.60
12		MOTA	2736			В	406	1.129 -10.294 35.878 1.00 23.65
10		ATOM	2737	CD CA	PRO	В	406	1.765 -12.632 36.148 1.00 25.91
34		ATOM	2738		PRO	В	406	1.899 -11.882 37.475 1.00 27.04
· Sani	L	MOTA	2739	CB	PRO	В	406	2.017 -10.431 37.068 1.00 26.56
***	\$	ATOM	2740	CG C	PRO PRO	В	406	0.876 -13.873 36.259 1.00 25.12
35		ATOM	2741 2742	0	PRO	В	406	1.368 -14.967 36.538 1.00 28.92
£150	35	MOTA	2742	N	ASN	В	407	-0.426 -13.713 36.039 1.00 23.53
1,4	ž.	ATOM ATOM	2743	CA	ASN	В	407	-1.345 -14.852 36.109 1.00 24.09
į,		ATOM	2744	CB	ASN	В	407	-2.553 -14.526 36.986 1.00 24.08
10		ATOM	2745	CG	ASN	В	407	-3.327 -13.328 36.486 1.00 26.72
1		ATOM	2747	OD1	ASN	В	407	-2.851 -12.574 35.635 1.00 22.65
1 2	40	ATOM	2748	ND2	ASN	В	407	-4.528 -13.140 37.019 1.00 26.46
	40	ATOM	2749	C	ASN	В	407	-1.820 -15.231 34.714 1.00 26.91
		ATOM	2750	0	ASN	В	407	-2.859 -15.870 34.548 1.00 28.68
		ATOM	275 1	N	LEU	В	408	-1.059 -14.816 33.708 1.00 27.28
		ATOM	2751	CA	LEU	В	408	-1.387 -15.124 32.327 1.00 27.23
	45	ATOM	2753	CB	LEU	В	408	-2.247 -14.030 31.699 1.00 26.61
	43	ATOM	2754	CG	LEU	В	408	-2.815 -14.464 30.341 1.00 27.51
		ATOM	2755	CD1	LEU	В	408	-3.702 -15.692 30.546 1.00 28.75
		ATOM	2756	CD2	LEU	В	408	-3.598 -13.330 29.694 1.00 25.48
		ATOM	2757	C	LEU	В	408	-0.113 -15.316 31.514 1.00 27.56
	50	ATOM	2758	0	LEU	В	408	0.247 -14.465 30.695 1.00 26.86
	50		2759	N	LEU	В	409	0.553 -16.426 31.759 1.00 27.54
		ATOM		CA	LEU	В	409	1.786 -16.774 31.065 1.00 31.96
		ATOM	2760	CB	LEU	В	409	2.786 -17.355 32.058 1.00 31.88
		ATOM	2761 2762	CG	LEU	В	409	4.186 -17.703 31.562 1.00 37.72
	55	ATOM		CD1	LEU	В	409	4.773 -16.551 30.770 1.00 39.57
	55	ATOM	2763 2764	CD1	LEU	В	409	5.066 -18.018 32.758 1.00 41.72
		ATOM	2765	C	LEU	В	409	1.401 -17.805 30.009 1.00 31.53
		ATOM		0	LEU	В	409	0.921 -18.892 30.340 1.00 32.67
		ATOM	2766 2767	N	LEU	В	410	1.604 -17.465 28.746 1.00 29.58
	60	ATOM ATOM	2768	CA	LEU	В	410	1.228 -18.361 27.660 1.00 31.55
	00	ATOM	2768	CB	LEU	В	410	0.192 -17.672 26.762 1.00 29.83
		ATOM	2770	CG	LEU	В	410	-1.047 -17.080 27.452 1.00 28.55
		MION	2110	CG	1111		-110	107

	_					_		-1.770 -16.135 26.501 1.00 26.92
	5	MOTA	2771	CD1	LEU	В	410	
		ATOM	2772	CD2	LEU	В	410	-1.979 -18.200 27.891 1.00 30.49
		MOTA	2773	C	LEU	В	410	2.397 -18.839 26.814 1.00 33.88
		ATOM	2774	0	LEU	В	410	3.427 -18.170 26.726 1.00 36.49
		ATOM	2775	N	ASP	В	411	2.238 -20.013 26.206 1.00 38.80
	10	ATOM	2776	CA	ASP	В	411	3.275 -20.562 25.336 1.00 38.39
		ATOM	2777	CB	ASP	В	411	3.657 -21.990 25.752 1.00 44.53
		MOTA	2778	CG	ASP	В	411	2.476 -22.943 25.749 1.00 44.90
			2779	OD1	ASP	В	411	1.773 -23.035 24.719 1.00 45.70
		MOTA						2.254 -23.603 26.786 1.00 50.54
		ATOM	2780	OD2	ASP	В	411	
	15	ATOM	2781	C	ASP	В	411	
		ATOM	2782	0	ASP	В	411	1.549 -20.341 23.686 1.00 36.48
		ATOM	2783	N	ARG	В	412	3.635 -20.777 22.949 1.00 36.85
		ATOM	2784	CA	ARG	В	412	3.259 -20.763 21.541 1.00 38.32
		ATOM	2785	CB	ARG	В	412	4.488 -21.083 20.675 1.00 38.69
	20	ATOM	2786	CG	ARG	В	412	4.361 -22.314 19.799 1.00 40.05
		ATOM	2787	CD	ARG	В	412	5.644 -22.552 19.012 1.00 42.98
		ATOM	2788	NE	ARG	В	412	5.540 -22.099 17.626 1.00 40.95
		ATOM	2789	CZ	ARG	В	412	4.649 -22.559 16.753 1.00 41.11
		ATOM	2790	NH1	ARG	В	412	3.777 -23.490 17.115 1.00 44.01
	25	ATOM	2791	NH2	ARG	В	412	4.632 -22.091 15.515 1.00 41.28
1.3	23			C		В	412	2.107 -21.712 21.217 1.00 37.64
13		ATOM	2792		ARG	В		1.287 -21.427 20.343 1.00 36.51
111		ATOM	2793	0	ARG		412	
133		ATOM	2794	N	ASN	В	413	
1 de		ATOM	2795	CA	ASN	В	413	0.974 -23.798 21.688 1.00 36.68
10.3	30	ATOM	2796	CB	ASN	В	413	1.170 -25.035 22.570 1.00 37.54
ş.in		MOTA	2797	CG	ASN	В	413	2.017 -26.100 21.901 1.00 43.56
1		ATOM	2798	OD1	ASN	В	413	2.309 -26.022 20.704 1.00 46.11
31		ATOM	2799	ND2	ASN	В	413	2.418 -27.104 22.671 1.00 47.04
		ATOM	2800	C	ASN	В	413	-0.383 -23.168 21.982 1.00 34.01
	35	MOTA	2801	0	ASN	В	413	-1.349 -23.372 21.247 1.00 32.43
لياية		MOTA	2802	N	GLN	В	414	-0.447 -22.397 23.063 1.00 32.85
100		ATOM	2803	CA	GLN	В	414	-1.685 -21.741 23.449 1.00 31.91
(1)		ATOM	2804	CB	GLN	В	414	-1.558 -21.172 24.863 1.00 33.17
11		ATOM	2805	CG	GLN	В	414	-1.528 -22.242 25.948 1.00 32.31
÷Ω	40		2806	CD	GLN	В	414	-1.293 -21.667 27.327 1.00 34.63
	40	MOTA		OE1	GLN	В	414	-0.176 -21.277 27.666 1.00 33.23
		MOTA	2807					-2.349 -21.606 28.131 1.00 34.56
		MOTA	2808	NE2	GLN	В	414	
		MOTA	2809	C	GLN	В	414	
		ATOM	2810	0	GLN	В	414	-3.195 -20.204 22.409 1.00 31.32
	45	MOTA	2811	N	GLY	В	415	-1.077 -20.190 21.682 1.00 30.96
		MOTA	2812	CA	GLY	В	415	-1.350 -19.160 20.697 1.00 34.27
		MOTA	2813	C	GLY	В	415	-2.184 -19.725 19.562 1.00 35.27
		ATOM	2814	0	GLY	В	415	-2.918 -19.000 18.887 1.00 33.20
		ATOM	2815	N	LYS	В	416	-2.070 -21.031 19.354 1.00 35.28
	50	ATOM	2816	CA	LYS	В	416	-2.819 -21.707 18.299 1.00 38.26
		ATOM	2817	CB	LYS	В	416	-2.398 -23.177 18.201 1.00 38.00
		ATOM	2818	CG	LYS	В	416	-0.973 -23.407 17.736 1.00 40.05
			2819	CD	LYS	В	416	-0.405 -24.668 18.369 1.00 44.10
		ATOM				В	416	0.306 -25.541 17.346 1.00 41.85
		ATOM	2820	CE	LYS			
	55	ATOM	2821		LYS	В	416	
		ATOM	2822		LYS	В	416	-4.321 -21.645 18.559 1.00 36.93
		MOTA	2823		LYS	В	416	-5.121 -21.790 17.638 1.00 38.36
		ATOM	2824		CYS	В	417	-4.698 -21.430 19.817 1.00 37.10
		MOTA	2825		CYS	В	417	-6.106 -21.371 20.196 1.00 36.46
	60	ATOM	2826	CB	CYS	В	417	-6.218 -21.226 21.717 1.00 39.01
		MOTA	2827	SG	CYS	В	417	-5.674 -22.710 22.612 1.00 43.81
		ATOM	2828	C	CYS	В	417	-6.899 -20.277 19.491 1.00 35.19
								4.00

	5	ATOM	2829	0	CYS	В	417	-8.127	-20.296	19.485	1.00	33.92
		ATOM	2830	N	VAL	В	418	-6.195	-19.316	18.906	1.00	36.04
		ATOM	2831	CA	VAL	В	418	-6.838	-18.236	18.163	1.00	34.59
		ATOM	2832	CB	VAL	В	418	-6.525	-16.850	18.775	1.00	34.87
		ATOM	2833	CG1	VAL	В	418	-6.831	-15.763	17.765	1.00	35.32
	10	ATOM	2834	CG2	VAL	В	418	-7.350	-16.630	20.036	1.00	33.65
	10	ATOM	2835	C	VAL	В	418		-18.317		1.00	34.17
		ATOM	2836	0	VAL	В	418		-18.323		1.00	32.73
				-	GLU	В	419		-18.388		1.00	33.44
		ATOM	2837	N		В	419		-18.500		1.00	34.52
	1.0	ATOM	2838	CA	GLU						1.00	36.21
	15	ATOM	2839	CB	GLU	В	419		-18.722			
		ATOM	2840	CG	GLU	В	419		-17.538		1.00	44.19
		ATOM	2841	CD	GLU	В	419		-17.723		1.00	48.47
		ATOM	2842	OE1	GLU	В	419		-18.605		1.00	51.04
		ATOM	2843	OE2	GLU	В	419	-10.484			1.00	48.91
	20	ATOM	2844	C	GLU	В	419		-17.289		1.00	32.89
		ATOM	2845	0	GLU	В	419	-6.156	-16.144	14.123	1.00	31.09
		ATOM	2846	N	GLY	В	420	-4.501	-17.562	13.535	1.00	32.84
		ATOM	2847	CA	GLY	В	420	-3.594	-16.506	13.122	1.00	34.37
		ATOM	2848	C	GLY	В	420	-2.722	-15.955	14.240	1.00	35.30
W125	25	ATOM	2849	Ō	GLY	В	420	-1.745	-15.246	13.975	1.00	35.94
120	25	ATOM	2850	N	MET	В	421		-16.285		1.00	30.08
10		ATOM	2851	CA	MET	В	421		-15.780		1.00	29.22
14		ATOM	2852	CB	MET	В	421		-15.922		1.00	22.54
1,53						В	421		-15.270		1.00	23.82
g: :: ú:	20	MOTA	2853	CG	MET		421		-13.494		1.00	28.40
h.i	30	ATOM	2854	SD	MET	В			-13.494		1.00	24.67
1200		MOTA	2855	CE	MET	В	421				1.00	29.67
4.		ATOM	2856	C	MET	В	421	-0.912	-16.416			29.76
3)		ATOM	2857	0	MET	В	421		-15.751		1.00	
125		ATOM	2858	N	VAL	В	422		-17.694		1.00	30.63
14	35	ATOM	2859	CA	VAL	В	422		-18.338		1.00	29.90
i.i		ATOM	2860	CB	VAL	В	422		-19.835		1.00	35.74
ü		ATOM	2861	CG1	VAL	В	422		-19.992		1.00	37.64
a di		MOTA	2862	CG2	VAL	В	422	1.659	-20.555		1.00	31.68
		ATOM	2863	C	VAL	В	422		-17.640		1.00	28.64
10	40	ATOM	2864	0	VAL	В	422	2.788	-17.571	16.441	1.00	26.15
		ATOM	2865	N	GLU	В	423	1.402	-17.113	14.747	1.00	28.70
		ATOM	2866	CA	GLU	В	423	2.454	-16.435	13.997	1.00	31.34
		ATOM	2867	CB	GLU	В	423	1.963	-16.050	12.596	1.00	36.21
		ATOM	2868	CG	GLU	В	423	0.502	-16.376	12.325	1.00	45.83
	45	ATOM	2869	CD	GLU	В	423	0.250	-17.865	12.144	1.00	46.71
		ATOM	2870	OE1	GLU	В	423	-0.746	-18.368	12.706	1.00	45.97
		ATOM	2871	OE2	GLU	В	423	1.045	-18.530		1.00	50.05
		ATOM	2872	C	GLU	В	423		-15.186		1.00	30.57
				0	GLU	В	423		-14.870		1.00	26.59
	50	ATOM	2873						-14.478		1.00	26.19
	50	ATOM	2874	N	ILE	В	424		-13.279		1.00	26.23
		ATOM	2875	CA	ILE	В	424	2.381			1.00	29.33
		MOTA	2876	CB	ILE	В	424		-12.435			
		ATOM	2877	CG2	ILE	В	424	1.492	-11.315		1.00	30.91
		ATOM	2878	CG1	ILE	В	424	0.584	-11.817		1.00	29.09
	55	ATOM	2879	CD1	ILE	В	424	-0.895	-11.514		1.00	30.51
		ATOM	2880	C	ILE	В	424	3.153	-13.673		1.00	24.22
		ATOM	2881	0	ILE	В	424	4.152	-13.037		1.00	21.05
		ATOM	2882	N	PHE	В	425	2.708	-14.746		1.00	21.71
		ATOM	2883	CA	PHE	В	425	3.370	-15.236		1.00	18.85
	60	ATOM	2884	CB	PHE	В	425	2.650	-16.479	19.768	1.00	22.98
		ATOM	2885	CG	PHE	В	425	1.580	-16.183	20.795	1.00	22.17
		ATOM	2886	CD1	PHE	В	425	1.287	-17.112	21.792	1.00	25.47
					_							

	5	ATOM	2887	CD2	PHE	В	425	0.843	-15.001 20.747	1.00	26.30
		ATOM	2888	CE1	PHE	В	425	0.273	-16.871 22.724	1.00	24.33
		ATOM	2889	CE2	PHE	В	425	-0.174	-14.749 21.676	1.00	25.03
		ATOM	2890	CZ	PHE	В	425	-0.459	-15.684 22.663	1.00	26.44
		ATOM	2891	C	PHE	В	425	4.817	-15.610 18.885	1.00	20.00
	10	ATOM	2892	ō	PHE	В	425		-15.292 19.636		21.15
		ATOM	2893	N	ASP	В	426	5.023	-16.281 17.754	1.00	19.87
		ATOM	2894	CA	ASP	В	426	6.378	-16.685 17.377		23.20
		ATOM	2895	CB	ASP	В	426		-17.510 16.090		26.53
			2896	CG	ASP	В	426		-18.965 16.335		34.28
	15	ATOM	2897	OD1	ASP	В	426	6.242	-19.467 17.455		35.24
	13	ATOM					426	5.448	-19.600 15.409		31.49
		ATOM	2898	OD2	ASP	В			-15.489 17.198		21.84
		MOTA	2899	C	ASP	В	426	7.302			
		ATOM	2900	0	ASP	В	426	8.465	-15.526 17.593		21.55
		ATOM	2901	N	MET	В	427		-14.429 16.591		20.12
	20	ATOM	2902	CA	MET	В	427		-13.234 16.382		21.02
		ATOM	2903	CB	MET	В	427		-12.228 15.520		18.53
		ATOM	2904	CG	MET	В	427		-12.559 14.038		27.92
		ATOM	2905	SD	MET	В	427		-11.341 13.024		32.84
		ATOM	2906	CE	MET	В	427	4.363	-11.532 13.581		33.63
	25	ATOM	2907	C	MET	В	427	7.945	-12.616 17.732	1.00	17.42
100		ATOM	2908	0	MET	В	427	9.073	-12.180 17.950	1.00	22.09
10		MOTA	2909	N	LEU	В	428	6.968	-12.597 18.634	1.00	20.47
		ATOM	2910	CA	LEU	В	428	7.157	-12.033 19.968	1.00	20.13
las las		ATOM	2911	CB	LEU	В	428	5.812	-11.964 20.706	1.00	17.58
324	30	ATOM	2912	CG	LEU	В	428	4.852	-10.887 20.179	1.00	18.41
lak lak		ATOM	2913	CD1	LEU	В	428	3.443	-11.155 20.687	7 1.00	11.95
And		ATOM	2914	CD2	LEU	В	428	5.324	-9.505 20.631	1.00	17.80
		ATOM	2915	C	LEU	В	428	8.159	-12.856 20.767		20.68
1)		ATOM	2916	ō	LEU	В	428		-12.305 21.445		20.45
(1)	35	ATOM	2917	N	LEU	В	429	8.037	-14.178 20.679		20.35
143	55	ATOM	2918	CA	LEU	В	429	8.938	-15.082 21.382		19.82
111		ATOM	2919	CB	LEU	В	429	8.470	-16.532 21.213		23.13
and mail		ATOM	2920	CG	LEU	В	429	7.189	-16.839 21.99		21.85
:D		ATOM	2921	CD1	LEU	В	429		-18.123 21.494		25.39
10	40	ATOM	2922	CD2	LEU	В	429		-16.944 23.475		24.91
	40	ATOM	2923	CDZ	LEU	В	429		-14.936 20.865		20.74
				0	LEU	В	429		-14.968 21.638		21.02
		ATOM	2924	N	ALA	В	430		-14.770 19.554		21.40
		ATOM	2925			В	430		-14.609 18.94		22.77
	45	ATOM	2926	CA	ALA				-14.596 17.432		21.11
	45	ATOM	2927	CB	ALA	В	430		-13.315 19.440		22.40
		ATOM	2928	C	ALA	В	430		-13.313 19.440		20.62
		ATOM	2929	0	ALA	В	430	13.670	-12.258 19.56		21.09
		ATOM	2930	N	THR	В	431	11.670			22.67
		ATOM	2931	CA	THR	В	431	12.183	-10.974 20.023		
	50	ATOM	2932	CB	THR	В	431	11.128	-9.866 19.863		23.77
		ATOM	2933	OG1	THR	В	431	10.572	-9.936 18.54		23.84
		ATOM	2934	CG2	THR	В	431	11.762	-8.489 20.073		21.78
		ATOM	2935	C	THR	В	431	12.603	-11.037 21.480		21.98
		ATOM	2936	0	THR	В	431	13.595	-10.429 21.87		19.85
	55	ATOM	2937	N	SER	В	432	11.844	-11.773 22.280		24.24
		ATOM	2938	CA	SER	В	432	12.169	-11.906 23.69		26.96
		ATOM	2939	CB	SER	В	432		-12.661 24.42		28.00
		ATOM	2940	OG	SER	В	432	11.404	-12.888 25.77		30.31
		ATOM	2941	C	SER	В	432	13.491	-12.660 23.82		27.67
	60	ATOM	2942	0	SER	В	432	14.305	-12.377 24.70		23.78
		ATOM	2943	N	SER	В	433	13.691	-13.628 22.93		29.27
		ATOM	2944	CA	SER	В	433	14.914	-14.421 22.928	3 1.00	31.96

	5	ATOM	2945	CB	SER	В	433	14.790	-15.575	21.938	1.00	30.84
		ATOM	2946	OG	SER	В	433	14.761	-16.808	22.625	1.00	38.26
		ATOM	2947	C	SER	В	433	16.104	-13.550	22.548	1.00	31.47
		ATOM	2948	0	SER	В	433	17.204	-13.701	23.087	1.00	28.43
		ATOM	2949	N	ARG	В	434	15.878	-12.641	21.607	1.00	29.55
	10	ATOM	2950	CA	ARG	В	434	16.926	-11.739		1.00	29.40
	10	ATOM	2951	CB	ARG	В	434	16.437	-10.912		1.00	31.56
		ATOM	2952	CG	ARG	В	434	17.428	-9.868		1.00	36.76
				CD		В	434	18.694	-10.502		1.00	37.76
		ATOM	2953		ARG			19.654	-9.479		1.00	39.50
	1.0	ATOM	2954	NE	ARG	В	434					
	15	ATOM	2955	CZ	ARG	В	434	20.965	-9.673		1.00	44.17
		ATOM	2956	NH1	ARG	В	434	21.492	-10.861		1.00	43.17
		ATOM	2957	NH2	ARG	В	434	21.750	-8.671		1.00	43.05
		MOTA	2958	C	ARG	В	434	17.328	-10.827		1.00	29.15
		ATOM	2959	0	ARG	В	434	18.515	-10.612		1.00	28.82
	20	ATOM	2960	N	PHE	В	435	16.337	-10.297	23.039	1.00	24.88
		ATOM	2961	CA	PHE	в	435	16.600	-9.422	24.186	1.00	25.74
		ATOM	2962	CB	PHE	В	435	15.278	-8.972	24.825	1.00	26.53
		ATOM	2963	CG	PHE	В	435	14.656	-7.758	24.183	1.00	30.94
		ATOM	2964	CD1	PHE	В	435	15.118	-7.271	22.966	1.00	32.65
	25	ATOM	2965	CD2	PHE	В	435	13.592	-7.108		1.00	33.60
(3	20	ATOM	2966	CE1	PHE	В	435	14.529		22.372	1.00	36.84
100		ATOM	2967	CE2	PHE	В	435	12.997		24.208	1.00	34.96
11		ATOM	2968	CZ	PHE	В	435	13.468		22.995	1.00	31.64
CO				C		В	435	17.426	-10.184		1.00	25.39
100	20	ATOM	2969		PHE			18.414		25.764	1.00	22.59
14	30	ATOM	2970	0	PHE	В	435	16.999	-11.405		1.00	24.58
- Seeler		ATOM	2971	N	ARG	В	436					
14		ATOM	2972	CA	ARG	В	436	17.675	-12.253		1.00	30.25
11		ATOM	2973	CB	ARG	В	436	16.898	-13.569		1.00	33.32
(1)		MOTA	2974	CG	ARG	В	436	17.232	-14.358		1.00	38.17
1,0	35	MOTA	2975	CD	ARG	В	436	16.135	-15.367		1.00	37.27
110		ATOM	2976	NE	ARG	В	436	15.646	-16.085		1.00	43.92
100		ATOM	2977	CZ	ARG	В	436	14.433			1.00	46.68
はは		MOTA	2978	NH1	ARG	В	436	13.578	-15.061		1.00	45.59
100		ATOM	2979	NH2	ARG	В	436	14.074	-16.620		1.00	46.25
ŧĐ.	40	ATOM	2980	C	ARG	В	436	19.110	-12.531	26.048	1.00	29.82
		ATOM	2981	0	ARG	В	436	20.057	-12.397	26.823	1.00	28.76
		ATOM	2982	N	AMET	В	437	19.269	-12.921	24.789	0.50	30.27
		ATOM	2983	N	BMET	В	437	19.252	-12.906	24.781	0.50	31.41
		ATOM	2984	CA	AMET	В	437	20.591	-13.212	24.253	0.50	31.98
	45	ATOM	2985	CA	BMET	В	437	20.547	-13.206	24.183	0.50	33.77
		ATOM	2986	CB	AMET	В	437	20.489	-13.646	22.788	0.50	31.34
		ATOM	2987	CB	BMET	В	437	20.348	-13.595		0.50	35.88
		ATOM	2988	CG	AMET	В	437	20.179	-15.127		0.50	33.62
		ATOM	2989	CG	BMET	В	437	21.605	-13.594		0.50	40.47
	50					_		20.354	-16.099		0.50	35.21
	30	MOTA	2990	SD	AMET	В	437		-13.937		0.50	46.79
		ATOM	2991	SD	BMET	В	437	21.247			0.50	33.20
		ATOM	2992	CE	AMET	В	437	22.155	-16.194			
		ATOM	2993	CE	BMET	В	437	21.837	-15.632		0.50	43.22
		MOTA	2994	C	AMET	В	437	21.498	-11.993		0.50	33.33
	55	MOTA	2995	C	BMET	В	437	21.487	-12.005		0.50	34.45
		ATOM	2996	0	AMET	В	437	22.702	-12.123		0.50	33.54
		ATOM	2997	0	BMET	В	437	22.699	-12.162	24.438	0.50	34.43
		ATOM	2998	N	MET	В	438	20.913	-10.809	24.215	1.00	32.07
		ATOM	2999	CA	MET	В	438	21.674	-9.560	24.298	1.00	32.48
	60	ATOM	3000	CB	MET	В	438	20.930	-8.437	23.578	1.00	29.74
		ATOM	3001	CG	MET	В	438	21.161	-8.364	22.093	1.00	36.73
		ATOM	3002	SD	MET	В	438	20.425		21.462	1.00	38.21

	5	ATOM	3003	CE	MET	В	438	21.693	-5.657 21.943	1.00	35.91
		ATOM	3004	C	MET	В	438	21.877	-9.122 25.738	1.00	28.81
		ATOM	3005	0	MET	В	438	22.686	-8.240 26.013	1.00	30.13
		ATOM	3006	N	ASN	В	439	21.120	-9.721 26.646	1.00	27.14
		ATOM	3007	CA	ASN	В	439	21.199	-9.359 28.038	1.00	27.34
	10	MOTA	3008	CB	ASN	В	439	22.592	-9.524 28.598	1.00	34.85
		ATOM	3009	CG	ASN	В	439	22.624	-9.480 30.080	1.00	38.58
		ATOM	3010	OD1	ASN	В	439	21.584	-9.620 30.724	1.00	42.99
		ATOM	3011	ND2	ASN	В	439	23.801	-9.260 30.666	1.00	41.14
		ATOM	3012	C	ASN	В	439	20.745	-7.903 28.212	1.00	26.24
	15		3012	0	ASN	В	439	21.396	-7.106 28.891	1.00	19.76
	13	ATOM							-7.564 27.573	1.00	24.90
		ATOM	3014	N	LEU	В	440	19.625			
		ATOM	3015	CA	LEU	В	440	19.061	-6.214 27.633	1.00	25.04
		ATOM	3016	CB	LEU	В	440	17.761	-6.157 26.818	1.00	22.36
		ATOM	3017	CG	LEU	В	440	17.087	-4.786 26.740	1.00	26.33
	20	MOTA	3018	CD1	LEU	В	440	17.958	-3.843 25.923	1.00	28.33
		MOTA	3019	CD2	LEU	В	440	15.704	-4.914 26.111	1.00	24.81
		ATOM	3020	C	LEU	В	440	18.782	-5.785 29.074	1.00	24.71
		ATOM	3021	0	LEU	В	440	18.131	-6.504 29.830	1.00	26.96
		ATOM	3022	N	GLN	В	441	19.268	-4.609 29.452	1.00	25.54
1180	25	MOTA	3023	CA	GLN	В	441	19.060	-4.099 30.807	1.00	25.82
144		ATOM	3024	CB	GLN	В	441	20.250	-3.231 31.234	1.00	30.41
10		MOTA	3025	CG	GLN	В	441	21.572	-3.956 31.228	1.00	30.50
2.56		ATOM	3026	CD	GLN	В	441	21.610	-5.028 32.279	1.00	32.75
0,13		ATOM	3027	OE1	GLN	В	441	21.539	-4.772 33.473	1.00	36.52
100		ATOM	3028	NE2	GLN	В	441	21.703	-6.288 31.823	1.00	31.09
1		ATOM	3029	C	GLN	В	441	17.789	-3.265 30.883	1.00	26.93
1.0		ATOM	3030	0	GLN	В	441	17.303	-2.768 29.866	1.00	25.40
14		ATOM	3031	N	GLY	В	442	17.266	-3.105 32.096	1.00	24.56
2		ATOM	3032	CA	GLY	В	442	16.058	-2.327 32.293	1.00	22.82
	35	ATOM	3032	C	GLY	В	442	16.217	-0.873 31.885	1.00	24.19
111	33		3033	0	GLY	В	442	15.290	-0.279 31.341	1.00	20.21
لِفا		ATOM				В	443	17.387	-0.293 32.141	1.00	22.92
1,1,1		MOTA	3035	N	GLU						23.33
12		MOTA	3036	CA	GLU	В	443	17.635	1.102 31.778	1.00	
147		MOTA	3037	CB	GLU	В	443	18.960	1.590 32.378	1.00	24.26
727	40	MOTA	3038	CG	GLU	В	443	19.005	1.525 33.895	1.00	32.31
		MOTA	3039	CD	GLU	В	443	19.701	0.270 34.402	1.00	37.68
		MOTA	3040	OE1	GLU	В	443	19.343	-0.841 33.948	1.00	35.23
		MOTA	3041	OE2	GLU	В	443	20.607	0.394 35.252	1.00	42.47
		MOTA	3042	C	GLU	В	443	17.662	1.278 30.262	1.00	23.08
	45	MOTA	3043	0	GLU	В	443	17.265	2.328 29.747	1.00	21.80
		MOTA	3044	N	GLU	В	444	18.128	0.253 29.552	1.00	21.16
		MOTA	3045	CA	GLU	В	444	18.182	0.302 28.093	1.00	22.60
		ATOM	3046	CB	GLU	В	444	19.046	-0.834 27.545	1.00	20.89
		ATOM	3047	CG	GLU	В	444	20.545	-0.617 27.705	1.00	23.24
	50	ATOM	3048	CD	GLU	В	444	21.340	-1.869 27.393	1.00	22.11
		ATOM	3049	OE1	GLU	В	444	20.817	-2.978 27.629	1.00	20.89
		ATOM	3050	OE2	GLU	В	444	22.488	-1.746 26.914	1.00	25.49
		ATOM	3051	C	GLU	В	444	16.758	0.155 27.552	1.00	21.06
		ATOM	3052	o	GLU	В	444	16.377	0.822 26.597	1.00	23.73
	55	ATOM	3053	N	PHE	В	445	15.987	-0.730 28.176	1.00	19.01
	55	ATOM	3054	CA	PHE	В	445	14.600	-0.969 27.792	1.00	19.44
						В	445	13.989	-2.067 28.675	1.00	18.12
		MOTA	3055	CB	PHE			12.483	-2.055 28.709	1.00	18.13
		ATOM	3056	CG CD1	PHE	B B	445 445	12.483	-2.055 28.709	1.00	18.34
	60	ATOM	3057	CD1	PHE			11.746	-1.694 29.872	1.00	16.59
	60	MOTA	3058	CD2	PHE	В	445				17.15
		MOTA	3059	CE1	PHE	В	445	10.346	-2.359 27.592	1.00	
		MOTA	3060	CE2	PHE	В	445	10.406	-1.662 29.903	1.00	21.99
								202			

	5	ATOM	3061	CZ	PHE	В	445	9.674	-1.997 28.755	1.00	16.01
		ATOM	3062	C	PHE	В	445	13.758	0.304 27.888	1.00	15.87
		ATOM	3063	0	PHE	В	445	13.008	0.617 26.966	1.00	20.27
		ATOM	3064	N	VAL	В	446	13.872	1.044 28.986	1.00	15.90
		ATOM	3065	CA	VAL	В	446	13.074	2.269 29.112	1.00	16.78
	10	ATOM	3066	CB	VAL	В	446	13.165	2.895 30.531	1.00	18.32
	10			CG1	VAL	В	446	12.574	1.923 31.551	1.00	21.14
		ATOM	3067			В	446	14.598	3.251 30.879	1.00	21.04
		ATOM	3068	CG2	VAL				3.295 28.051	1.00	17.91
		ATOM	3069	C	VAL	В	446	13.450			19.37
		ATOM	3070	0	VAL	В	446	12.596	4.028 27.561	1.00	
	15	ATOM	3071	N	CYS	В	447	14.723	3.335 27.674	1.00	18.81
		MOTA	3072	CA	CYS	В	447	15.161	4.255 26.635	1.00	17.34
		MOTA	3073	CB	CYS	В	447	16.682	4.224 26.512	1.00	19.33
		MOTA	3074	SG	CYS	В	447	17.538	5.134 27.798	1.00	23.60
		ATOM	3075	C	CYS	В	447	14.537	3.826 25.301	1.00	18.09
	20	ATOM	3076	0	CYS	В	447	13.988	4.643 24.563	1.00	17.52
		ATOM	3077	N	LEU	В	448	14.623	2.533 25.006	1.00	15.60
		ATOM	3078	CA	LEU	В	448	14.072	1.994 23.767	1.00	16.67
		ATOM	3079	CB	LEU	В	448	14.328	0.490 23.684	1.00	14.82
		ATOM	3080	CG	LEU	В	448	15.730	0.009 23.301	1.00	23.57
/554	25	ATOM	3081	CD1	LEU	В	448	15.722	-1.522 23.169	1.00	21.61
(7)		ATOM	3082	CD2	LEU	В	448	16.167	0.658 21.986	1.00	18.92
102		ATOM	3083	C	LEU	В	448	12.573	2.249 23.652	1.00	15.98
14		ATOM	3084	0	LEU	В	448	12.078	2.633 22.590	1.00	18.91
琐			3085	N	LYS	В	449	11.849	2.037 24.745	1.00	17.94
(chi	30	ATOM		CA		В	449	10.405	2.232 24.733	1.00	16.66
34.3	30	ATOM	3086	CB	LYS	В	449	9.796	1.745 26.047	1.00	16.45
100		ATOM	3087		LYS			8.285	1.861 26.115	1.00	16.12
14		ATOM	3088	CG	LYS	В	449	7.730	0.952 27.193	1.00	19.09
41		ATOM	3089	CD	LYS	В	449			1.00	17.04
(2)		ATOM	3090	CE	LYS	В	449	8.201	1.380 28.580		17.25
1,15	35	MOTA	3091	NZ	LYS	В	449	7.159	1.088 29.593	1.00	
1,1		ATOM	3092	C	LYS	В	449	10.058	3.696 24.486	1.00	18.78
110		MOTA	3093	0	LYS	В	449	9.103	3.996 23.769	1.00	14.84
40		MOTA	3094	N	SER	В	450	10.837	4.610 25.059	1.00	14.50
10		ATOM	3095	CA	SER	В	450	10.591	6.032 24.849	1.00	17.11
1975	40	MOTA	3096	CB	SER	В	450	11.440	6.866 25.815	1.00	21.20
		ATOM	3097	OG	SER	В	450	10.859	6.868 27.108	1.00	30.66
		ATOM	3098	C	SER	В	450	10.921	6.418 23.405	1.00	17.84
		ATOM	3099	0	SER	В	450	10.279	7.292 22.821	1.00	18.82
		ATOM	3100	N	ILE	В	451	11.926	5.768 22.828	1.00	16.88
	45	ATOM	3101	CA	ILE	В	451	12.305	6.063 21.450	1.00	17.11
		ATOM	3102	CB	ILE	В	451	13.564	5.268 21.025	1.00	16.69
		ATOM	3103	CG2	ILE	В	451	13.724	5.298 19.505	1.00	19.31
		ATOM	3104	CG1	ILE	В	451	14.804	5.897 21.676	1.00	18.96
		ATOM	3105	CD1	ILE	В	451	16.083	5.130 21.431	1.00	18.98
	50	ATOM	3106	C	ILE	В	451	11.142	5.711 20.527	1.00	18.09
	50	ATOM	3107	0	ILE	В	451	10.820	6.464 19.608	1.00	17.07
		ATOM	3108	N	ILE	В	452	10.505	4.571 20.786	1.00	18.13
				CA	ILE	В	452	9.373	4.137 19.976	1.00	16.77
		ATOM	3109					8.804	2.775 20.477	1.00	17.40
		ATOM	3110	CB	ILE	В	452	7.464	2.496 19.831	1.00	14.33
	55	ATOM	3111	CG2	ILE	В	452		1.635 20.107	1.00	15.36
		ATOM	3112	CG1	ILE	В	452	9.763			
		ATOM	3113	CD1	ILE	В	452	9.449	0.323 20.805	1.00	17.76
		ATOM	3114	C	ILE	В	452	8.271	5.195 20.024	1.00	17.47
		ATOM	3115	0	ILE	В	452	7.733	5.586 18.992	1.00	16.50
	60	ATOM	3116	N	LEU	В	453	7.943	5.665 21.222	1.00	16.06
		ATOM	3117	CA	LEU	В	453	6.903	6.680 21.374	1.00	17.17
		ATOM	3118	CB	LEU	В	453	6.736	7.061 22.850	1.00	16.23

	5	ATOM	3119	CG	LEU	В	453	5.792	8.228 23.163	1.00	17.60
		ATOM	3120	CD1	LEU	В	453	4.388	7.881 22.704	1.00	16.94
		ATOM	3121	CD2	LEU	В	453	5.816	8.538 24.667	1.00	17.17
		MOTA	3122	C	LEU	В	453	7.198	7.941 20.566	1.00	19.33
		ATOM	3123	0	LEU	В	453	6.320	8.458 19.879	1.00	21.37
	10	ATOM	3124	N	LEU	В	454	8.434	8.428 20.636	1.00	17.68
		ATOM	3125	CA	LEU	В	454	8.789	9.653 19.933	1.00	20.93
		ATOM	3126	CB	LEU	В	454	9.959	10.347 20.653	1.00	24.33
		ATOM	3127	CG	LEU	В	454	9.735	10.699 22.130	1.00	26.16
		ATOM	3128	CD1	LEU	В	454	11.046	11.170 22.749	1.00	24.82
	15	ATOM	3129	CD2	LEU	В	454	8.658	11.777 22.259	1.00	23.79
		ATOM	3130	C	LEU	В	454	9.120	9.494 18.449	1.00	20.75
		ATOM	3131	o	LEU	В	454	8.941	10.431 17.673	1.00	21.33
		ATOM	3132	N	ASN	В	455	9.566	8.311 18.042	1.00	20.54
		ATOM	3133	CA	ASN	В	455	9.951	8.093 16.651	1.00	19.46
	20	ATOM	3134	CB	ASN	В	455	11.147	7.149 16.584	1.00	18.58
	20	ATOM	3135	CG	ASN	В	455	11.576	6.871 15.161	1.00	17.64
		ATOM	3136	OD1	ASN	В	455	12.106	7.749 14.496	1.00	18.40
		ATOM	3137	ND2	ASN	В	455	11.343	5.648 14.686	1.00	15.06
		ATOM	3138	C	ASN	В	455	8.925	7.580 15.655	1.00	22.77
	25	ATOM	3139	0	ASN	В	455	8.790	8.127 14.564	1.00	21.94
10	23	ATOM	3140	N	SER	В	456	8.224	6.514 16.023	1.00	25.90
+0		ATOM	3141	CA	SER	В	456	7.260	5.873 15.135	1.00	24.76
14		ATOM	3142	CB	SER	В	456	6.402	4.894 15.939	1.00	26.91
170			3143	OG	SER	В	456	7.212	3.818 16.390	1.00	26.24
į mb	30	MOTA MOTA	3143	C	SER	В	456	6.385	6.774 14.272	1.00	26.52
14	30		3145	0	SER	В	456	6.323	6.588 13.055	1.00	29.22
inch.		MOTA	3145	N	GLY	В	457	5.716	7.750 14.872	1.00	22.07
1		MOTA	3145	CA	GLY	В	457	4.879	8.627 14.076	1.00	25.19
31		ATOM ATOM	3148	CA	GLY	В	457	5.510	9.973 13.765	1.00	28.59
(10)	35	ATOM	3149	0	GLY	В	457	4.851	10.850 13.214	1.00	28.31
1.1	33	ATOM	3150	N	VAL	В	458	6.789	10.130 14.092	1.00	31.65
1.1		ATOM	3151	CA	VAL	В	458	7.486	11.396 13.879	1.00	38.50
17		ATOM	3151	CB	VAL	В	458	8.950	11.310 14.373	1.00	36.24
10		ATOM	3152	CG1	VAL	В	458	9.827	10.650 13.324	1.00	38.50
1	40	ATOM	3154	CG2	VAL	В	458	9.463	12.699 14.701	1.00	39.84
	40	ATOM	3154	C	VAL	В	458	7.483	11.982 12.464	1.00	46.30
		ATOM	3156	0	VAL	В	458	7.567	13.201 12.302	1.00	47.67
		ATOM	3157	N	TYR	В	459	7.393	11.138 11.442	1.00	50.45
		ATOM	3157	CA	TYR	В	459	7.385	11.640 10.069	1.00	57.07
	45		3159	CB	TYR	В	459	8.233	10.740 9.170	1.00	57.05
	43	ATOM ATOM	3160	CG	TYR	В	459	9.673	10.680 9.611	1.00	59.29
			3161	CD1	TYR	В	459	10.284	11.786 10.203	1.00	60.93
		ATOM	3162	CE1	TYR	В	459	11.591	11.725 10.662	1.00	61.86
		ATOM		CD2	TYR	В	459	10.414	9.510 9.486	1.00	59.46
		MOTA	3163					11.726	9.439 9.943	1.00	59.67
	50	ATOM	3164	CE2	TYR	В	459	12.305	10.548 10.532	1.00	60.84
		ATOM	3165	CZ	TYR	В	459		10.477 11.009	1.00	61.39
		ATOM	3166	OH	TYR	В	459	13.593		1.00	61.22
		MOTA	3167	С	TYR	В	459	5.976		1.00	62.89
		ATOM	3168	0	TYR	В	459	5.629			
	55	MOTA	3169	N	THR	В	460	5.166	10.730 9.768	1.00	65.15
		ATOM	3170	CA	THR	В	460	3.783	10.702 9.309		67.76
		MOTA	3171	CB	THR	В	460	3.178	9.283 9.464		68.02
		ATOM	3172	OG1	THR	В	460	1.890	9.235 8.836		67.03
		ATOM	3173	CG2	THR	В	460	3.040	8.916 10.938		67.31
	60	MOTA	3174	C	THR	В	460	2.945	11.700 10.107		70.14
		ATOM	3175	0	THR	В	460	1.715	11.641 10.099		72.35
		ATOM	3176	N	PHE	в	461	3.625	12.620 10.788	1.00	72.64

	5	ATOM	3177	CA	PHE	В	461	2.969	13.637 11.607	1.00	75.05
		ATOM	3178	CB	PHE	В	461	3.977	14.720 12.012	1.00	75.47
		ATOM	3179	CG	PHE	В	461	4.235	14.789 13.492	1.00	74.32
		ATOM	3180	CD1	PHE	В	461	3.200	14.609 14.404	1.00	73.98
		ATOM	3181	CD2	PHE	В	461	5.517	15.025 13.975	1.00	75.22
	10	ATOM	3182	CE1	PHE	В	461	3.438	14.662 15.775	1.00	74.02
	10	ATOM	3183	CE2	PHE	В	461	5.765	15.080 15.344	1.00	74.50
			3184	CZ	PHE	В	461	4.722	14.897 16.245	1.00	74.10
		ATOM				В	461	1.787	14.286 10.896	1.00	76.78
		ATOM	3185	C	PHE				14.279 9.645	1.00	77.08
		ATOM	3186	0	PHE	В	461	1.775			
	15	ATOM	3187	CB	GLU	В	470	7.873	23.789 14.718	1.00	80.19
		ATOM	3188	C	GLU	В	470	8.958	21.731 15.650	1.00	79.30
		ATOM	3189	0	GLU	В	470	9.887	21.518 16.432	1.00	78.21
		MOTA	3190	N	GLU	В	470	9.096	22.235 13.227	1.00	80.22
		ATOM	3191	CA	GLU	В	470	9.060	22.830 14.595	1.00	80.03
	20	ATOM	3192	N	GLU	В	471	7.823	21.037 15.665	1.00	78.31
		ATOM	3193	CA	GLU	В	471	7.596	19.956 16.617	1.00	75.83
		ATOM	3194	CB	GLU	В	471	6.118	19.543 16.604	1.00	76.70
		ATOM	3195	CG	GLU	В	471	5.742	18.544 15.516	1.00	78.42
		ATOM	3196	CD	GLU	В	471	5.062	19.198 14.327	1.00	79.69
1000	25	ATOM	3197	OE1	GLU	В	471	3.829	19.398 14.378	1.00	80.26
10	20	ATOM	3198	OE2	GLU	В	471	5.763	19.511 13.340	1.00	80.72
TÚ		ATOM	3199	C	GLU	В	471	8.487	18.756 16.292	1.00	73.13
10		ATOM	3200	0	GLU	В	471	8.897	18.021 17.189	1.00	73.86
10			3201	N	LYS	В	472	8.785	18.565 15.009	1.00	69.65
- Justi	30	ATOM		CA	LYS	В	472	9.639	17.461 14.581	1.00	64.40
14	30	ATOM	3202			В	472	9.578	17.293 13.060	1.00	63.78
lech:		MOTA	3203	CB	LYS				16.552 12.566	1.00	64.49
1		MOTA	3204	CG	LYS	В	472	8.343	16.002 11.161	1.00	63.81
1		ATOM	3205	CD	LYS	В	472	8.544		1.00	64.90
\$125 \$125		MOTA	3206	CE	LYS	В	472	7.379	16.368 10.249		
1,1	35	ATOM	3207	NZ	LYS	В	472	6.475	15.212 9.990	1.00	63.97
1.1		MOTA	3208	C	LYS	В	472	11.071	17.749 15.014	1.00	61.03
		MOTA	3209	0	LYS	В	472	11.848	16.833 15.287	1.00	60.28
10		ATOM	3210	N	ASP	В	473	11.413	19.033 15.076	1.00	56.84
		ATOM	3211	CA	ASP	В	473	12.745	19.451 15.488	1.00	51.69
D	40	ATOM	3212	CB	ASP	В	473	12.923	20.940 15.242	1.00	50.36
		ATOM	3213	C	ASP	В	473	12.923	19.138 16.970	1.00	49.18
		ATOM	3214	0	ASP	В	473	13.959	18.619 17.385	1.00	46.85
		ATOM	3215	N	HIS	В	474	11.898	19.449 17.758	1.00	45.35
		ATOM	3216	CA	HIS	В	474	11.923	19.203 19.196	1.00	43.65
	45	ATOM	3217	CB	HIS	В	474	10.652	19.761 19.847	1.00	43.70
		ATOM	3218	CG	HIS	В	474	10.458	19.326 21.267	1.00	43.86
		MOTA	3219	CD2	HIS	В	474	11.095	19.688 22.406	1.00	44.12
		ATOM	3220	ND1	HIS	В	474	9.510	18.395 21.638	1.00	46.60
		ATOM	3221	CE1	HIS	В	474	9.572	18.202 22.943	1.00	45.29
	50	ATOM	3222	NE2	HIS	В	474	10.526	18.975 23.434	1.00	47.96
	50	ATOM	3223	C	HIS	В	474	12.030	17.707 19.471	1.00	42.38
			3224	0	HIS	В	474	12.834	17.273 20.298	1.00	42.83
		ATOM				В	475	11.214	16.923 18.773	1.00	38.86
		ATOM	3225	N	ILE				15.475 18.943	1.00	36.53
		ATOM	3226	CA	ILE	В	475	11.222			36.56
	55	MOTA	3227	CB	ILE	В	475	10.105	14.822 18.110	1.00	
		ATOM	3228	CG2	ILE	В	475	10.390	13.335 17.911	1.00	36.17
		MOTA	3229	CG1	ILE	В	475	8.770	14.998 18.832	1.00	35.81
		MOTA	3230	CD1	ILE	В	475	7.598	14.410 18.094	1.00	41.77
		ATOM	3231	C	ILE	В	475	12.575	14.898 18.532	1.00	33.72
	60	ATOM	3232	0	ILE	В	475	13.112	14.023 19.207	1.00	31.50
		MOTA	3233	N	HIS	В	476	13.121	15.375 17.429	1.00	33.65
		ATOM	3234	CA	HIS	В	476	14.421	14.886 16.992	1.00	33.31

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	5	ATOM	3235	CB	HIS	В	476	14.782	15.481 15.637	1.00	37.30
		ATOM	3236	CG	HIS	В	476	14.132	14.781 14.486	1.00	43.64
		ATOM	3237	CD2	HIS	В	476	13.723	13.498 14.342	1.00	45.25
		ATOM	3238	ND1	HIS	В	476	13.816	15.419 13.306	1.00	48.37
						В	476	13.238	14.560 12.484	1.00	48.87
		ATOM	3239	CE1	HIS						
	10	ATOM	3240	NE2	HIS	В	476	13.170	13.387 13.089	1.00	48.11
		ATOM	3241	C	HIS	В	476	15.506	15.213 18.022	1.00	31.20
		ATOM	3242	0	HIS	В	476	16.442	14.436 18.208	1.00	27.25
		ATOM	3243	N	ARG	В	477	15.387	16.365 18.684	1.00	30.64
		ATOM	3244	CA	ARG	В	477	16.361	16.754 19.703	1.00	30.09
	15							16.144	18.214 20.121	1.00	33.46
	13	ATOM	3245	CB	ARG	В	477				
		ATOM	3246	CG	ARG	В	477	16.322	19.212 18.982	1.00	40.74
		MOTA	3247	CD	ARG	В	477	16.274	20.649 19.479	1.00	45.91
		MOTA	3248	NE	ARG	В	477	17.514	21.020 20.155	1.00	51.37
		ATOM	3249	CZ	ARG	В	477	18.375	21.927 19.702	1.00	53.68
	20	ATOM	3250	NH1	ARG	В	477	18.140	22.567 18.560	1.00	53.04
		ATOM	3251	NH2	ARG	В	477	19.480	22.185 20.389	1.00	51.79
		ATOM	3252	C	ARG	В	477	16.232	15.835 20.925	1.00	26.97
		ATOM	3253	0	ARG	В	477	17.233	15.387 21.486	1.00	27.34
									15.558 21.338	1.00	23.70
	2.5	MOTA	3254	N	VAL	В	478	14.999			
(200)	25	ATOM	3255	CA	VAL	В	478	14.780	14.685 22.482	1.00	24.79
-0		ATOM	3256	CB	VAL	В	478	13.286	14.613 22.861	1.00	24.83
ıÜ		ATOM	3257	CG1	VAL	В	478	13.088	13.646 24.022	1.00	26.23
10		MOTA	3258	CG2	VAL	В	478	12.781	15.996 23.243	1.00	28.26
5,4,5		ATOM	3259	C	VAL	В	478	15.284	13.294 22.112	1.00	26.10
- Frede	30	ATOM	3260	0	VAL	В	478	15.919	12.613 22.927	1.00	24.28
24		ATOM	3261	N	LEU	В	479	15.021	12.889 20.870	1.00	22.92
Salak		ATOM	3262	CA	LEU	В	479	15.456	11.584 20.379	1.00	21.96
10					LEU	В	479	14.992	11.372 18.930	1.00	22.63
31		ATOM	3263	CB					10.798 18.756	1.00	20.82
0		MOTA	3264	CG	LEU	В	479	13.575			
1 _k J	35	MOTA	3265	CD1	LEU	В	479	13.231	10.689 17.274	1.00	22.53
W		MOTA	3266	CD2	LEU	В	479	13.495	9.440 19.420	1.00	23.08
555		ATOM	3267	C	LEU	В	479	16.975	11.471 20.453	1.00	21.90
12		MOTA	3268	0	LEU	В	479	17.506	10.416 20.778	1.00	23.11
- 50		ATOM	3269	N	ASP	В	480	17.675	12.560 20.143	1.00	23.65
10	40	ATOM	3270	CA	ASP	В	480	19.141	12.566 20.198	1.00	24.29
	10	ATOM	3271	CB	ASP	В	480	19.692	13.889 19.649	1.00	26.88
				CG	ASP	В	480	19.773	13.914 18.129	1.00	33.32
		ATOM	3272								35.44
		MOTA	3273	OD1	ASP	В	480	19.857	12.836 17.499	1.00	
		MOTA	3274	OD2	ASP	В	480	19.757	15.022 17.563	1.00	32.44
	45	MOTA	3275	C	ASP	В	480	19.590	12.406 21.656	1.00	24.13
		ATOM	3276	0	ASP	В	480	20.551	11.697 21.956	1.00	24.88
		ATOM	3277	N	LYS	В	481	18.887	13.077 22.560	1.00	25.18
		MOTA	3278	CA	LYS	В	481	19.213	13.010 23.980	1.00	26.78
		ATOM	3279	CB	LYS	В	481	18.262	13.898 24.785	1.00	31.37
	50	ATOM	3280	CG	LYS	В	481	18.962	14.788 25.804	1.00	43.84
	50	ATOM	3281	CD	LYS	В	481	18.780	14.260 27.219	1.00	46.08
									13.928 27.865	1.00	50.99
		MOTA	3282	CE	LYS	В	481	20.120			
		ATOM	3283	NZ	LYS	В	481	21.177	14.922 27.511	1.00	54.35
		ATOM	3284	C	LYS	В	481	19.124	11.575 24.495	1.00	26.87
	55	ATOM	3285	0	LYS	В	481	19.951	11.145 25.305	1.00	20.37
		ATOM	3286	N	ILE	В	482	18.124	10.830 24.027	1.00	23.26
		ATOM	3287	CA	ILE	В	482	17.981	9.452 24.472	1.00	21.07
		ATOM	3288	CB	ILE	В	482	16.655	8.828 24.015	1.00	19.80
		ATOM	3289	CG2	ILE	В	482	16.580	7.370 24.491	1.00	17.40
	60	ATOM	3290	CG1	ILE	В	482	15.479	9.606 24.602	1.00	17.16
	00		3290	CD1	ILE	В	482	14.136	9.209 23.991	1.00	19.43
		ATOM							8.616 23.947	1.00	20.21
		ATOM	3292	С	ILE	В	482	19.135	0.010 43.94/	1.00	20.21

	5	ATOM	3293	0	ILE	В	482	19.621	7.722 24.640	1.00	25.55
	,			N	THR	В	483	19.569	8.896 22.722	1.00	21.89
		ATOM	3294			В	483	20.701	8.176 22.141	1.00	22.67
		ATOM	3295	CA	THR				8.662 20.695	1.00	23.34
		ATOM	3296	CB	THR	В	483	21.030			27.33
		ATOM	3297	OG1	THR	В	483	19.890	8.475 19.851	1.00	
	10	ATOM	3298	CG2	THR	В	483	22.203	7.882 20.116	1.00	24.46
		ATOM	3299	C	THR	В	483	21.913	8.441 23.035	1.00	23.51
		ATOM	3300	0	THR	В	483	22.650	7.520 23.381	1.00	27.01
		ATOM	3301	N	ASP	В	484	22.119	9.703 23.404	1.00	22.88
		ATOM	3302	CA	ASP	В	484	23.237	10.058 24.276	1.00	24.93
	15	ATOM	3303	CB	ASP	В	484	23.201	11.546 24.652	1.00	28.69
		ATOM	3304	CG	ASP	В	484	23.504	12.464 23.485	1.00	29.19
		ATOM	3305	OD1	ASP	В	484	23.982	11.984 22.437	1.00	29.63
		ATOM	3306	OD2	ASP	В	484	23.256	13.681 23.627	1.00	32.02
		ATOM	3307	C	ASP	в	484	23.125	9.249 25.567	1.00	24.40
	20	ATOM	3308	ō	ASP	В	484	24.125	8.780 26.103	1.00	25.60
	20	ATOM	3309	N	THR	В	485	21.899	9.096 26.066	1.00	20.16
		ATOM	3310	CA	THR	В	485	21.670	8.365 27.307	1.00	22.28
		ATOM	3311	CB	THR	В	485	20.203	8.521 27.763	1.00	24.64
						В	485	19.878	9.914 27.830	1.00	24.28
	25	ATOM	3312	OG1	THR				7.896 29.133	1.00	23.32
(1)	25	ATOM	3313	CG2	THR	В	485	19.993	6.881 27.188	1.00	22.13
100		ATOM	3314	C	THR	В	485	22.017			23.30
111		ATOM	3315	0	THR	В	485	22.574	6.284 28.115	1.00	
10		ATOM	3316	N	LEU	В	486	21.686	6.290 26.045	1.00	23.08
14		ATOM	3317	CA	LEU	В	486	21.969	4.881 25.792	1.00	22.26
14	30	ATOM	3318	CB	LEU	В	486	21.346	4.452 24.464	1.00	20.93
1.4		MOTA	3319	CG	LEU	В	486	19.878	4.031 24.533	1.00	24.92
i.		ATOM	3320	CD1	LEU	В	486	19.295	4.003 23.123	1.00	21.96
- 10		MOTA	3321	CD2	LEU	В	486	19.763	2.658 25.196	1.00	23.90
100		ATOM	3322	C	LEU	В	486	23.477	4.634 25.742	1.00	24.12
Li	35	ATOM	3323	0	LEU	В	486	23.984	3.681 26.334	1.00	24.02
Li		ATOM	3324	N	ILE	В	487	24.191	5.490 25.022	1.00	24.53
13		ATOM	3325	CA	ILE	В	487	25.640	5.345 24.913	1.00	25.16
F120		ATOM	3326	CB	ILE	В	487	26.207	6.379 23.899	1.00	25.57
15		ATOM	3327	CG2	ILE	В	487	27.725	6.522 24.051	1.00	24.54
123	40	ATOM	3328	CG1	ILE	В	487	25.857	5.936 22.470	1.00	25.63
		ATOM	3329	CD1	ILE	В	487	26.538	4.646 22.021	1.00	25.68
		ATOM	3330	C	ILE	В	487	26.275	5.518 26.307	1.00	23.60
		ATOM	3331	0	ILE	В	487	27.200	4.794 26.671	1.00	23.65
		ATOM	3332	N	HIS	В	488	25.755	6.456 27.081	1.00	21.75
	45	ATOM	3333	CA	HIS	В	488	26.251	6.720 28.431	1.00	26.07
		ATOM	3334	CB	HIS	В	488	25.450	7.871 29.041	1.00	26.99
		ATOM	3335	CG	HIS	В	488	25.818	8.196 30.455	1.00	33.06
		ATOM	3336	CD2	HIS	В	488	25.245	7.838 31.629	1.00	32.79
		ATOM	3337	ND1	HIS	В	488	26.869	9.025 30.779	1.00	36.45
	50	ATOM	3338	CE1	HIS	В	488	26.927	9.164 32.091	1.00	35.93
	30		3339	NE2	HIS	В	488	25.953	8.453 32.630	1.00	33.88
		ATOM				В	488	26.123	5.463 29.292	1.00	26.85
		ATOM	3340	C	HIS				5.054 29.967	1.00	28.52
		ATOM	3341	0	HIS	В	488	27.071	4.850 29.266	1.00	28.00
		ATOM	3342	N	LEU	В	489	24.949			
	55	ATOM	3343	CA	LEU	В	489	24.715	3.642 30.040	1.00	25.94
		ATOM	3344	CB	LEU	В	489	23.298	3.127 29.788	1.00	27.07
		ATOM	3345	CG	LEU	В	489	22.158	3.909 30.445	1.00	31.71
		ATOM	3346	CD1	LEU	В	489	20.827	3.516 29.799	1.00	28.08
		ATOM	3347	CD2	LEU	В	489	22.143	3.616 31.949	1.00	29.30
	60	ATOM	3348	C	LEU	В	489	25.718	2.561 29.642	1.00	26.84
		ATOM	3349	0	LEU	В	489	26.241	1.832 30.486	1.00	20.86
		ATOM	3350	N	MET	В	490	25.978	2.453 28.345	1.00	23.82
								205			

	5	ATOM	3351	CA	MET	В	490	26.900	1.438 27.857	1.00	26.38
		ATOM	3352	CB	MET	В	490	26.775	1.306 26.336	1.00	27.29
		ATOM	3353	CG	MET	В	490	25.418	0.776 25.895	1.00	21.68
		ATOM	3354	SD	MET	В	490	25.208	0.739 24.106	1.00	26.30
		ATOM	3355	CE	MET	В	490	23.461	0.412 24.022	1.00	19.66
	10	ATOM	3356	C	MET	В	490	28.341	1.743 28.247	1.00	26.42
		ATOM	3357	0	MET	В	490	29.109	0.833 28.574	1.00	24.76
		ATOM	3358	N	ALA	В	491	28.713	3.018 28.207	1.00	26.67
		ATOM	3359	CA	ALA	В	491	30.074	3.394 28.577	1.00	30.73
		ATOM	3360	CB	ALA	В	491	30.299	4.882 28.335	1.00	26.66
	15		3361	С	ALA	В	491	30.250	3.053 30.056	1.00	32.08
	13	ATOM		0	ALA	В	491	31.194	2.361 30.438	1.00	34.66
		ATOM	3362				492	29.316	3.523 30.878	1.00	33.17
		ATOM	3363	N	LYS	В		29.316	3.267 32.309	1.00	32.82
		ATOM	3364	CA	LYS	В	492		3.849 32.976	1.00	36.38
	20	ATOM	3365	CB	LYS	В	492	28.110			38.68
	20	ATOM	3366	CG	LYS	В	492	28.412	4.797 34.123	1.00	41.41
		ATOM	3367	CD	LYS	В	492	27.242	4.887 35.084	1.00	
		ATOM	3368	CE	LYS	В	492	26.299	6.013 34.698	1.00	47.57
		ATOM	3369	NZ	LYS	В	492	26.395	7.184 35.618	1.00	50.76
		ATOM	3370	C	LYS	В	492	29.453	1.771 32.619	1.00	34.08
į.	25	MOTA	3371	0	LYS	В	492	30.090	1.382 33.593	1.00	34.31
4	17	MOTA	3372	N	ALA	В	493	28.835	0.935 31.788	1.00	32.03
į.	11	MOTA	3373	CA	ALA	В	493	28.867	-0.510 31.998	1.00	30.70
2	2 23 2 2 1 1	MOTA	3374	CB	ALA	В	493	27.719	-1.181 31.245	1.00	28.80
-	## 20	ATOM	3375	C	ALA	В	493	30.201	-1.156 31.606	1.00	33.75
- 1	30	ATOM	3376	0	ALA	В	493	30.402	-2.356 31.819	1.00	30.53
		ATOM	3377	N	GLY	В	494	31.102	-0.372 31.020	1.00	33.50
	ed.	ATOM	3378	CA	GLY	В	494	32.405	-0.903 30.656	1.00	33.71
	ų.	ATOM	3379	C	GLY	В	494	32.639	-1.360 29.230	1.00	34.40
		ATOM	3380	0	GLY	В	494	33.663	-1.989 28.950	1.00	33.13
8	35	ATOM	3381	N	LEU	В	495	31.712	-1.056 28.326	1.00	31.76
8	Ail .	ATOM	3382	CA	LEU	В	495	31.859	-1.452 26.925	1.00	30.57
3	u)	ATOM	3383	CB	LEU	В	495	30.494	-1.415 26.216	1.00	30.67
Ā	3	ATOM	3384	CG	LEU	В	495	29.610	-2.675 26.256	1.00	29.59
1	Ð	ATOM	3385	CD1	LEU	В	495	29.315	-3.058 27.700	1.00	26.60
4	□ 40	ATOM	3386	CD2	LEU	В	495	28.307	-2.416 25.501	1.00	27.52
	70	ATOM	3387	C	LEU	В	495	32.829	-0.515 26.202	1.00	30.53
		ATOM	3388	ō	LEU	В	495	32.855	0.688 26.468	1.00	28.14
		ATOM	3389	N	THR	В	496	33.628	-1.064 25.291	1.00	28.03
		ATOM	3390	CA	THR	В	496	34.567	-0.243 24.529	1.00	29.06
	45	ATOM	3391	CB	THR	В	496	35.511	-1.095 23.665	1.00	29.40
	73		3392	OG1	THR	В	496	34.753	-1.758 22.641	1.00	30.29
		ATOM		CG2	THR	В	496	36.228	-2.122 24.515	1.00	28.12
		ATOM	3393		THR	В	496	33.770	0.652 23.590	1.00	30.12
		ATOM	3394	C				32.580	0.433 23.380	1.00	29.74
		MOTA	3395	0	THR	В	496		1.654 23.018	1.00	30.44
	50	ATOM	3396	N	LEU	В	497	34.430	2.567 22.104	1.00	28.54
		MOTA	3397	CA	LEU	В	497	33.762			31.14
		ATOM	3398	CB	LEU	В	497	34.768	3.564 21.529	1.00	
		ATOM	3399	CG	LEU	В	497	35.209	4.719 22.434	1.00	33.58
		ATOM	3400	CD1	LEU	В	497	36.120	5.659 21.652	1.00	31.42
	55	ATOM	3401	CD2	LEU	В	497	33.992	5.469 22.942	1.00	35.08
		MOTA	3402	C	LEU	В	497	33.095	1.800 20.967	1.00	27.35
		ATOM	3403	0	LEU	В	497	31.967	2.105 20.574	1.00	24.03
		ATOM	3404	N	GLN	В	498	33.798	0.797 20.447	1.00	26.17
		ATOM	3405	CA	GLN	В	498	33.289	-0.009 19.348	1.00	26.32
	60	ATOM	3406	CB	GLN	В	498	34.411	-0.876 18.771	1.00	27.25
		ATOM	3407	CG	GLN	В	498	33.967	-1.796 17.645	1.00	32.67
		MOTA	3408	CD	GLN	В	498	34.965	-2.912 17.374	1.00	38.39
								200			

	5	ATOM	3409	OE1	GLN	В	498	35.737	-3.298 18.254	1.00	36.78
		ATOM	3410	NE2	GLN	В	498	34.953	-3.437 16.153	1.00	33.18
		ATOM	3411	C	GLN	В	498	32.112	-0.888 19.774	1.00	25.70
		MOTA	3412	0	GLN	В	498	31.167	-1.076 19.009	1.00	25.35
		ATOM	3413	N	GLN	В	499	32.173	-1.434 20.986	1.00	24.01
1		ATOM	3414	CA	GLN	В	499	31.093	-2.281 21.487	1.00	25.34
1	U			CB	GLN	В	499	31.501	-2.935 22.815	1.00	28.38
		ATOM	3415				499	32.537	-4.056 22.669	1.00	29.13
		ATOM	3416	CG	GLN	В		32.913	-4.687 23.995	1.00	30.80
		ATOM	3417	CD	GLN	В	499				33.62
	_	ATOM	3418	OE1	GLN	В	499	33.306	-3.997 24.937	1.00	
1	5	ATOM	3419	NE2	GLN	В	499	32.797	-6.004 24.074	1.00	30.64
		ATOM	3420	C	GLN	В	499	29.842	-1.430 21.693	1.00	25.70
		ATOM	3421	0	GLN	В	499	28.715	-1.910 21.554	1.00	26.22
		ATOM	3422	N	GLN	В	500	30.062	-0.160 22.020	1.00	23.09
		ATOM	3423	CA	GLN	В	500	28.989	0.793 22.256	1.00	23.53
2	0	ATOM	3424	CB	GLN	В	500	29.564	2.107 22.782	1.00	26.17
		ATOM	3425	CG	GLN	В	500	29.958	2.073 24.252	1.00	27.71
		ATOM	3426	CD	GLN	В	500	30.812	3.262 24.641	1.00	29.32
		ATOM	3427	OE1	GLN	В	500	30.559	4.386 24.207	1.00	28.48
		ATOM	3428	NE2	GLN	В	500	31.831	3.021 25.463	1.00	25.07
2	.5		3429	C	GLN	В	500	28.151	1.074 21.015	1.00	24.24
South	.5	ATOM		0	GLN	В	500	26.923	0.949 21.053	1.00	24.40
10		ATOM	3430					28.790	1.465 19.915	1.00	23.08
L		MOTA	3431	N	HIS	В	501		1.739 18.724	1.00	26.92
(10		ATOM	3432	CA	HIS	В	501	28.004			
Beach		MOTA	3433	CB	HIS	В	501	28.791	2.577 17.697	1.00	32.00
3	0	MOTA	3434	CG	HIS	В	501	29.988	1.896 17.105	1.00	36.97
rain .		ATOM	3435	CD2	HIS	В	501	30.122	0.710 16.465	1.00	40.32
14		MOTA	3436	ND1	HIS	В	501	31.224	2.505 17.042	1.00	37.88
¥1		ATOM	3437	CE1	HIS	В	501	32.066	1.724 16.389	1.00	38.81
(m) 2		ATOM	3438	NE2	HIS	В	501	31.422	0.628 16.028	1.00	41.21
3	5	ATOM	3439	C	HIS	В	501	27.451	0.457 18.123	1.00	25.91
1AJ		ATOM	3440	0	HIS	В	501	26.369	0.457 17.531	1.00	20.13
W		ATOM	3441	N	GLN	В	502	28.165	-0.648 18.317	1.00	24.94
(12.2)		ATOM	3442	CA	GLN	В	502	27.698	-1.926 17.804	1.00	21.88
\$ 1985 1985		ATOM	3443	CB	GLN	В	502	28.785	-2.996 17.953	1.00	24.62
·Ø 4	10	ATOM	3444	CG	GLN	В	502	29.796	-3.001 16.797	1.00	26.55
		ATOM	3445	CD	GLN	В	502	30.843	-4.109 16.902	1.00	27.06
		ATOM	3446	OE1	GLN	В	502	30.716	-5.033 17.705	1.00	28.49
		ATOM	3447	NE2	GLN	В	502	31.882	-4.018 16.078	1.00	21.90
		ATOM	3448	C	GLN	В	502	26.428	-2.341 18.554	1.00	22.39
,	15			0	GLN	В	502	25.464	-2.807 17.944	1.00	22.24
4	+3	ATOM	3449			В	503	26.421	-2.159 19.874	1.00	20.54
		ATOM	3450	N	ARG			25.259	-2.523 20.678	1.00	22.04
		ATOM	3451	CA	ARG	В	503		-2.519 22.180	1.00	22.51
		ATOM	3452	CB	ARG	В	503	25.602			23.34
_		ATOM	3453	CG	ARG	В	503	24.451	-3.022 23.077	1.00	
5	50	MOTA	3454	CD	ARG	В	503	24.853	-3.110 24.550	1.00	22.18
		ATOM	3455	NE	ARG	В	503	23.743	-3.546 25.395	1.00	19.62
		MOTA	3456	CZ	ARG	В	503	23.329	-4.807 25.497	1.00	19.88
		ATOM	3457	NH1	ARG	В	503	23.933	-5.765 24.809	1.00	16.40
		ATOM	3458	NH2	ARG	В	503	22.303	-5.110 26.280	1.00	19.71
5	55	ATOM	3459	C	ARG	В	503	24.102	-1.558 20.409	1.00	19.05
		ATOM	3460	0	ARG	В	503	22.945	-1.968 20.351	1.00	18.87
		ATOM	3461	N	LEU	В	504	24.414	-0.276 20.239	1.00	20.19
		ATOM	3462	CA	LEU	В	504	23.375	0.714 19.969	1.00	19.33
		ATOM	3463	CB	LEU	В	504	23.972	2.117 19.855	1.00	16.25
	50	ATOM	3464	CG	LEU	В	504	22.983	3.173 19.344	1.00	20.35
,	,,,	ATOM	3465	CD1	LEU	В	504	21.930	3.449 20.427	1.00	17.97
					LEU	В	504	23.729	4.448 18.955	1.00	20.86
		ATOM	3466	CD2	TPC	ь	JU4	23.129	4.440 10.933	1.00	20.00

		_			_		_		0.0	659	0 255	18.667	1.00	21.22
		5	ATOM	3467	C	LEU	В	504						
			ATOM	3468	0	LEU	В	504		433		18.566	1.00	19.28
			ATOM	3469	N	ALA	В	505		428		17.676	1.00	18.55
			ATOM	3470	CA	ALA	В	505		859	-0.473		1.00	18.20
			ATOM	3471	CB	ALA	В	505	23.	973	-0.745	15.382	1.00	18.45
	1	10	ATOM	3472	C	ALA	В	505	21.	986	-1.716	16.562	1.00	19.54
			ATOM	3473	0	ALA	В	505	20.	871	-1.774	16.041	1.00	17.63
			ATOM	3474	N	GLN	В	506		497	-2.706	17.293	1.00	20.30
			ATOM	3475	CA	GLN	В	506		772	-3.955	17.513	1.00	19.48
			ATOM	3476	CB	GLN	В	506		590		18.409	1.00	21.75
	1	15	ATOM	3477	CG	GLN	В	506		798		17.727	1.00	20.85
		LJ					В	506		819		18.736	1.00	26.18
			ATOM	3478	CD	GLN						19.943	1.00	21.83
			MOTA	3479	OE1	GLN	В	506		564				
			ATOM	3480	NE2	GLN	В	506		977		18.245	1.00	25.39
			ATOM	3481	C	GLN	В	506		421		18.166	1.00	21.39
	2	20	ATOM	3482	0	GLN	В	506		396		17.766	1.00	20.87
			MOTA	3483	N	LEU	В	507		433		19.171	1.00	19.52
			ATOM	3484	CA	LEU	В	507	19.	219	-2.418	19.884	1.00	23.04
			ATOM	3485	CB	LEU	В	507	19.	548	-1.455	21.030	1.00	22.82
			ATOM	3486	CG	LEU	В	507	20.	182	-2.011	22.313	1.00	26.12
	iss 2	25	ATOM	3487	CD1	LEU	В	507	20.	203	-0.916	23.360	1.00	29.33
-	1022		ATOM	3488	CD2	LEU	В	507		415		22.816	1.00	27.80
1	Ø.		ATOM	3489	C	LEU	В	507		212		18.971	1.00	22.19
-	U		ATOM	3490	0	LEU	В	507		036		18.964	1.00	23.00
	ij.				N	LEU	В	508		678		18.214	1.00	21.53
	nå ,	20	ATOM	3491								17.332	1.00	20.60
	4	30	MOTA	3492	CA	LEU	В	508		797				
	last.		MOTA	3493	CB	LEU	В	508		.535		16.805	1.00	17.57
-	1		MOTA	3494	CG	LEU	В	508		934		17.913	1.00	17.67
	1		MOTA	3495	CD1	LEU	В	508		.566		17.301	1.00	20.04
			ATOM	3496	CD2	LEU	В	508	17.	724		18.725	1.00	18.49
-	107	35	ATOM	3497	C	LEU	В	508	17.	. 235		16.183	1.00	21.17
	id.		ATOM	3498	0	LEU	В	508	16.	.118	-0.597	15.728	1.00	21.88
-	100		ATOM	3499	N	LEU	В	509	18.	.000	-1.813	15.713	1.00	21.89
			ATOM	3500	CA	LEU	В	509	17.	511	-2.657	14.631	1.00	22.81
	Ď.		ATOM	3501	CB	LEU	В	509	18.	603	-3.597	14.145	1.00	22.65
-	D 2	40	ATOM	3502	CG	LEU	В	509	19.	645	-2.891	13.278	1.00	29.11
			ATOM	3503	CD1	LEU	В	509		697	-3.888	12.829	1.00	25.69
			ATOM	3504	CD2	LEU	В	509		965		12.082	1.00	27.92
			ATOM	3505	C	LEU	В	509		302		15.095	1.00	23.32
						LEU	В	509		.409		14.303	1.00	23.36
		45	MOTA	3506	0			510		.264		16.380	1.00	23.36
	-	43	MOTA	3507	N	ILE	В						1.00	20.99
			MOTA	3508	CA	ILE	В	510		.148		16.912		
			ATOM	3509	CB	ILE	В	510		.448		18.361	1.00	28.60
			ATOM	3510	CG2	ILE	В	510		.162		19.075	1.00	28.10
			ATOM	3511	CG1	ILE	В	510		.383		18.308	1.00	26.57
		50	ATOM	3512	CD1	ILE	В	510	17.	.429	-6.301	19.419	1.00	30.14
			ATOM	3513	C	ILE	В	510	13.	.852	-3.746	16.846	1.00	17.65
			ATOM	3514	0	ILE	В	510	12.	.767	-4.308	16.759	1.00	16.11
			ATOM	3515	N	LEU	В	511		.961	-2.421	16.867	1.00	18.12
			ATOM	3516	CA	LEU	В	511		.772		16.774	1.00	16.95
		55	ATOM	3517	CB	LEU	В	511		147		16.981	1.00	22.66
		55					В			607		18.406	1.00	22.13
			ATOM	3518	CG	LEU		511						25.29
			ATOM	3519	CD1	LEU	В	511		.404		18.652	1.00	
			ATOM	3520	CD2	LEU	В	511		.830		19.425	1.00	25.08
			ATOM	3521	C	LEU	В	511		.112		15.397	1.00	16.65
	-	60	MOTA	3522	0	LEU	В	511		.915		15.242	1.00	17.09
			ATOM	3523	N	SER	В	512		.901		14.401	1.00	15.83
			ATOM	3524	CA	SER	В	512	12.	. 355	-2.408	13.072	1.00	18.66

	5	ATOM	3525	CB	SER	В	512	13.484	-2.644 12.074	1.00	17.62
		ATOM	3526	OG	SER	В	512	13.079	-3.550 11.062	1.00	32.77
		ATOM	3527	C	SER	В	512	11.454	-3.638 13.154	1.00	18.54
		ATOM	3528	0	SER	В	512	10.373	-3.683 12.545	1.00	17.01
		ATOM	3529	N	HIS	В	513	11.899	-4.625 13.929	1.00	15.54
	10	MOTA	3530	CA	HIS	В	513	11.141	-5.860 14.115	1.00	17.67
		ATOM	3531	CB	HIS	В	513	12.013	-6.916 14.790	1.00	19.03
		ATOM	3532	CG	HIS	В	513	13.063	-7.475 13.886	1.00	27.06
		ATOM	3533	CD2	HIS	В	513	12.980	-8.364 12.868	1.00	28.40
		ATOM	3534	ND1	HIS	В	513	14.378	-7.066 13.932	1.00	28.92
	15	ATOM	3535	CE1	HIS	В	513	15.061	-7.678 12.981	1.00	30.75
		ATOM	3536	NE2	HIS	В	513	14.235	-8.472 12.321	1.00	30.08
		MOTA	3537	C	HIS	В	513	9.895	-5.602 14.958	1.00	15.35
		ATOM	3538	0	HIS	В	513	8.846	-6.192 14.704	1.00	14.83
		ATOM	3539	N	ILE	В	514	10.012	-4.744 15.942	1.00	13.35
	20	ATOM	3540	CA	ILE	В	514	8.865	-4.417 16.776	1.00	15.48
		ATOM	3541	CB	ILE	В	514	9.295	-3.534 17.967	1.00	20.02
		ATOM	3542	CG2	ILE	В	514	8.067	-2.918 18.650	1.00	12.84
		ATOM	3543	CG1	ILE	В	514	10.093	-4.397 18.962	1.00	22.87
		ATOM	3544	CD1	ILE	В	514	10.691	-3.641 20.115	1.00	29.62
	25	ATOM	3545	C	ILE	В	514	7.797	-3.717 15.923	1.00	15.16
]	20	ATOM	3546	0	ILE	В	514	6.606	-3.972 16.078	1.00	16.61
3		ATOM	3547	N	ARG	В	515	8.224	-2.823 15.030	1.00	16.33
1		ATOM	3548	CA	ARG	В	515	7.280	-2.138 14.150	1.00	17.54
0		ATOM	3549	CB	ARG	В	515	8.010	-1.173 13.214	1.00	20.15
site	30	ATOM	3550	CG	ARG	В	515	7.080	-0.454 12.234	1.00	21.47
· j	50	ATOM	3551	CD	ARG	В	515	6.407	0.749 12.891	1.00	26.05
sk		ATOM	3552	NE	ARG	В	515	7.220	1.948 12.716	1.00	24.91
ŝ		ATOM	3553	CZ	ARG	В	515	6.734	3.175 12.547	1.00	24.61
		ATOM	3554	NH1	ARG	В	515	5.424	3.393 12.522	1.00	22.46
200	35	ATOM	3555	NH2	ARG	В	515	7.569	4.182 12.374	1.00	23.15
	55	ATOM	3556	C	ARG	В	515	6.545	-3.182 13.304	1.00	16.60
1 2 2 2		ATOM	3557	0	ARG	В	515	5.332	-3.093 13.087	1.00	14.51
10 14		ATOM	3558	N	HIS	В	516	7.298	-4.171 12.827	1.00	18.50
do,		ATOM	3559	CA	HIS	В	516	6.743	-5.237 11.997	1.00	17.26
Ĩ.	40	ATOM	3560	CB	HIS	В	516	7.861	-6.176 11.533	1.00	18.14
	40	ATOM	3561	CG	HIS	В	516	7.405	-7.223 10.568	1.00	24.87
		ATOM	3562	CD2	HIS	В	516	7.060	-8.521 10.754	1.00	26.64
		ATOM	3563	ND1	HIS	В	516	7.258	-6.978 9.220	1.00	21.82
		ATOM	3564	CE1	HIS	В	516	6.839	-8.078 8.619	1.00	28.42
	45	ATOM	3565	NE2	HIS	В	516	6.711	-9.028 9.526	1.00	24.47
	+3	ATOM	3566	C	HIS	В	516	5.685	-6.028 12.759	1.00	16.87
		ATOM	3567	0	HIS	В	516	4.596	-6.303 12.240	1.00	14.81
			3568	N	MET	В	517	5.999	-6.396 13.997	1.00	16.48
		MOTA	3569	CA	MET	В	517	5.049	-7.162 14.801	1.00	15.39
	50	ATOM	3570	CB	MET	В	517	5.701	-7.587 16.114	1.00	21.05
	50	ATOM		CG	MET	В	517	6.790	-8.638 15.917	1.00	20.76
		ATOM	3571	SD	MET	В	517	7.380	-9.320 17.470	1.00	23.96
		ATOM	3572			В	517	8.104	-7.879 18.226	1.00	20.45
		ATOM	3573	CE	MET MET	В	517	3.789	-6.368 15.080	1.00	16.23
	<i>E E</i>	ATOM	3574					2.688	-6.924 15.148	1.00	16.02
	55	ATOM	3575	0	MET	В	517		-5.060 15.247	1.00	13.32
		ATOM	3576	N	SER	В	518	3.954 2.827	-5.060 15.247 -4.186 15.505	1.00	16.34
		ATOM	3577	CA	SER	В	518			1.00	17.48
		ATOM	3578	CB	SER	В	518	3.316	-2.765 15.835		17.46
		ATOM	3579	OG	SER	В	518	2.234	-1.840 15.843	1.00	
	60	ATOM	3580	C	SER	В	518	1.906	-4.147 14.284	1.00	14.73
		ATOM	3581	0	SER	В	518	0.688	-4.247 14.417	1.00	19.16
		ATOM	3582	N	ASN	В	519	2.474	-4.006 13.091	1.00	14.52
								211			

	5	ATOM	3583	CA	ASN	В	519	1.622	-3.953	11.907	1.00	15.35
		ATOM	3584	CB	ASN	В	519	2.432	-3.509	10.698	1.00	19.21
		ATOM	3585	CG	ASN	В	519	2.700	-2.029	10.729	1.00	20.58
		ATOM	3586	OD1	ASN	В	519	1.839	-1.258	11.150	1.00	26.36
		ATOM	3587	ND2	ASN	В	519	3.891	-1.618		1.00	19.62
	10			C	ASN	В	519	0.911	-5.280		1.00	16.74
	10	ATOM	3588						-5.299		1.00	20.58
		MOTA	3589	0	ASN	В	519	-0.265				
		ATOM	3590	N	LYS	В	520	1.608	-6.387		1.00	18.60
		ATOM	3591	CA	LYS	В	520	0.992	-7.699		1.00	20.04
		ATOM	3592	CB	LYS	В	520	2.038	-8.801		1.00	25.44
	15	MOTA	3593	CG	LYS	В	520	3.037	-8.849		1.00	31.68
		MOTA	3594	CD	LYS	В	520	2.507	-9.663	9.558	1.00	42.56
		MOTA	3595	CE	LYS	В	520	2.186	-8.778	8.364	1.00	45.61
		MOTA	3596	NZ	LYS	В	520	1.435	-9.526	7.312	1.00	46.00
		ATOM	3597	C	LYS	В	520	-0.099	-7.868	12.769	1.00	18.88
	20	ATOM	3598	0	LYS	В	520	-1.183	-8.358	12.478	1.00	21.75
		ATOM	3599	N	GLY	В	521	0.191	-7.455	13.998	1.00	17.83
		MOTA	3600	CA	GLY	В	521	-0.792	-7.569	15.058	1.00	16.19
		MOTA	3601	C	GLY	В	521	-2.000	-6.674	14.833	1.00	16.59
		ATOM	3602	o	GLY	В	521	-3.128	-7.060		1.00	16.57
	25	ATOM	3603	N	MET	В	522	-1.766	-5.467		1.00	17.48
1,3	23	ATOM	3604	CA	MET	В	522	-2.852	-4.527		1.00	18.25
10		ATOM	3605	CB	MET	В	522	-2.276	-3.212		1.00	21.27
11								-3.190	-2.018		1.00	26.97
77		MOTA	3606	CG	MET	В	522					30.35
2.08)	20	ATOM	3607	SD	MET	В	522	-3.199	-1.477		1.00	
1	30	MOTA	3608	CE	MET	В	522	-1.659	-0.605		1.00	29.86
1.2		ATOM	3609	C	MET	В	522	-3.794	-5.119		1.00	18.68
14.3		ATOM	3610	0	MET	В	522	-5.022	-5.008		1.00	18.80
51		MOTA	3611	N	GLU	В	523	-3.205	-5.731		1.00	18.22
[7]		ATOM	3612	CA	GLU	В	523	-3.968	-6.357		1.00	23.41
Lu	35	MOTA	3613	CB	GLU	В	523	-3.031	-6.946	9.830	1.00	28.74
W		MOTA	3614	CG	GLU	В	523	-2.224	-5.935	9.030	1.00	34.42
124		MOTA	3615	CD	GLU	В	523	-1.095	-6.597	8.239	1.00	45.58
£120		MOTA	3616	OE1	GLU	В	523	-0.131	-5.894	7.857	1.00	49.48
123		ATOM	3617	OE2	GLU	В	523	-1.169	-7.825	7.999	1.00	45.97
ıΔ	40	MOTA	3618	C	GLU	В	523	-4.812	-7.482	11.465	1.00	23.98
		ATOM	3619	0	GLU	В	523	-5.993	-7.616	11.147	1.00	22.08
		ATOM	3620	N	HIS	В	524	-4.187	-8.287	12.326	1.00	23.46
		ATOM	3621	CA	HIS	В	524	-4.846	-9.428	12.952	1.00	26.20
		ATOM	3622	CB	HIS	В	524	-3.824	-10.245	13.743	1.00	27.26
	45	ATOM	3623	CG	HIS	В	524	-4.378	-11.509		1.00	30.91
	75	ATOM	3624	CD2	HIS	В	524	-4.308	-12.792		1.00	30.90
		ATOM	3625	ND1	HIS	В	524	-5.107	-11.537		1.00	28.87
		ATOM	3625	CE1	HIS	В	524	-5.461	-12.780		1.00	30.45
			3627	NE2	HIS	В	524	-4.989	-13.561		1.00	29.19
	50	ATOM						-5.996	-9.025		1.00	27.69
	50	MOTA	3628	C	HIS	В	524	-7.061	-9.656		1.00	25.00
		ATOM	3629	0	HIS	В	524					23.84
		ATOM	3630	N	LEU	В	525	-5.777	-7.977		1.00	
		MOTA	3631	CA	LEU	В	525	-6.786	-7.492		1.00	25.77
		ATOM	3632	CB	LEU	В	525	-6.217	-6.358		1.00	22.22
	55	MOTA	3633	CG	LEU	В	525	-7.164	-5.778		1.00	26.81
		ATOM	3634	CD1	LEU	В	525	-7.763	-6.922		1.00	23.32
		ATOM	3635	CD2	LEU	В	525	-6.414	-4.793		1.00	18.95
		ATOM	3636	C	LEU	В	525	-8.013	-6.995	14.842	1.00	26.84
		ATOM	3637	0	LEU	В	525	-9.154	-7.247	15.249	1.00	26.73
	60	ATOM	3638	N	TYR	В	526	-7.764	-6.271	13.757	1.00	26.86
		ATOM	3639	CA	TYR	В	526	-8.819	-5.726	12.918	1.00	30.89
		ATOM	3640	CB	TYR	В	526	-8.201	-4.818		1.00	34.31
								212				
								212				

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	5	MOTA	3641	CG	TYR	В	526	-9.183		10.878	1.00	43.50
		ATOM	3642	CD1	TYR	В	526	-10.058		11.267	1.00	47.66
		ATOM	3643	CE1	TYR	В	526	-10.943	-2.636	10.357	1.00	48.85
		ATOM	3644	CD2	TYR	В	526	-9.218	-4.651	9.552	1.00	48.52
		ATOM	3645	CE2	TYR	В	526	-10.098	-4.083	8.634	1.00	52.43
	10	ATOM	3646	CZ	TYR	В	526	-10.955	-3.077	9.043	1.00	51.67
	10			OH		В	526	-11.810	-2.504	8.129	1.00	57.01
		MOTA	3647		TYR							
		MOTA	3648	C	TYR	В	526	-9.577		12.265	1.00	30.90
		ATOM	3649	0	TYR	В	526	-10.793		12.113	1.00	31.48
		ATOM	3650	N	SER	В	527	-8.849		11.889	1.00	31.39
	15	ATOM	3651	CA	SER	В	527	-9.460	-9.095	11.266	1.00	33.73
		ATOM	3652	CB	SER	В	527	-8.377	-10.048	10.749	1.00	34.13
		ATOM	3653	OG	SER	В	527	-8.945	-11.222	10.196	1.00	43.67
		ATOM	3654	C	SER	В	527	-10.339		12.288	1.00	34.34
		ATOM	3655	0	SER	В	527	-11.446	-10.261		1.00	33.42
	20							-9.840		13.517	1.00	31.66
	20	ATOM	3656	N	MET	В	528					
		ATOM	3657	CA	MET	В	528	-10.574	-10.572		1.00	29.77
		ATOM	3658	CB	MET	В	528	-9.682	-10.743	15.820	1.00	32.96
		ATOM	3659	CG	MET	В	528	-8.651	-11.859	15.699	1.00	33.47
		ATOM	3660	SD	MET	В	528	-9.359	-13.427	15.134	1.00	38.28
2200	25	MOTA	3661	CE	MET	В	528	-10.265	-13.915	16.579	1.00	36.01
100		ATOM	3662	C	MET	В	528	-11.800		14.953	1.00	29.42
40		ATOM	3663	o	MET	В	528	-12.835	-10.293		1.00	28.65
('U		ATOM	3664	N	LYS	В	529	-11.673		14.850	1.00	30.64
10										15.149	1.00	31.80
ini.	••	MOTA	3665	CA	LYS	В	529	-12.781				
Mil	30	ATOM	3666	CB	LYS	В	529	-12.323		15.027	1.00	32.86
i nis		ATOM	3667	CG	LYS	В	529	-13.436		15.114	1.00	36.42
14		MOTA	3668	CD	LYS	В	529	-13.114	-3.852	14.224	1.00	41.74
8		ATOM	3669	CE	LYS	В	529	-13.734	-2.564	14.741	1.00	43.45
-79%		ATOM	3670	NZ	LYS	В	529	-15.221	-2.569	14.634	1.00	46.51
103	35	ATOM	3671	C	LYS	В	529	-13.857	-7.840	14.116	1.00	36.60
116		ATOM	3672	ō	LYS	В	529	-15.049		14.424	1.00	34.04
14		ATOM	3673	N	CYS	В	530	-13.407		12.889	1.00	40.04
(23				CA	CYS	В	530	-14.286		11.773	1.00	44.58
10		ATOM	3674					-14.260		10.491		50.64
163	40	ATOM	3675	CB	CYS	В	530				1.00	
1997	40	ATOM	3676	SG	CYS	В	530	-13.369	-7.034	9.504	1.00	67.65
		ATOM	3677	C	CYS	В	530	-15.065		12.016	1.00	42.88
		ATOM	3678	0	CYS	В	530	-16.274		11.807	1.00	40.15
		ATOM	3679	N	LYS	В	531	-14.360	-10.733	12.447	1.00	41.92
		ATOM	3680	CA	LYS	В	531	-14.980	-12.023	12.728	1.00	42.60
	45	ATOM	3681	CB	LYS	В	531	-13.907	-13.091	12.927	1.00	44.77
		MOTA	3682	C	LYS	В	531	-15.844	-11.907	13.977	1.00	44.43
		ATOM	3683	0	LYS	В	531	-16.623	-12.804		1.00	44.09
		ATOM	3684	N	ASN	В	532	-15.678	-10.793		1.00	44.98
								-16.437	-10.795		1.00	44.10
		ATOM	3685	CA	ASN	В	532					
	50	ATOM	3686	CB	ASN	В	532	-17.833	-10.003		1.00	45.14
		MOTA	3687	CG	ASN	В	532	-18.526		16.633	1.00	46.54
		ATOM	3688	OD1	ASN	В	532	-19.729	-9.424	16.837	1.00	50.62
		ATOM	3689	ND2	ASN	В	532	-17.771	-8.471	17.375	1.00	46.07
		ATOM	3690	C	ASN	В	532	-16.557	-11.657	16.882	1.00	43.34
	55	ATOM	3691	o	ASN	В	532		-11.994		1.00	41.42
	55	ATOM	3692	N	VAL	В	533	-15.434	-12.264		1.00	43.45
									-13.371		1.00	44.06
		ATOM	3693	CA	VAL	В	533					
		ATOM	3694	CB	VAL	В	533		-14.219		1.00	45.56
		ATOM	3695	CG1	VAL	В	533	-13.661	-14.263		1.00	45.67
	60	MOTA	3696	CG2	VAL	В	533	-13.107	-13.644		1.00	44.16
		ATOM	3697	C	VAL	В	533		-12.835		1.00	43.24
		ATOM	3698	0	VAL	В	533	-15.894	-13.602	20.548	1.00	44.21

	5	ATOM	3699	N	VAL	В	534		-11.511		1.00	40.44
		ATOM	3700	CA	VAL	В	534	-15.765	-10.849	21.049	1.00	37.80
		ATOM	3701	CB	VAL	В	534	-14.630	-11.259	22.038	1.00	36.38
		MOTA	3702	CG1	VAL	В	534	-13.324	-10.575		1.00	34.35
		ATOM	3703	CG2	VAL	В	534	-15.021	-10.910	23.463	1.00	39.34
	10	MOTA	3704	С	VAL	В	534	-15.752	-9.329	20.857	1.00	37.97
		ATOM	3705	0	VAL	В	534	-15.026	-8.808	20.008	1.00	39.45
		ATOM	3706	N	PRO	В	535	-16.575	-8.597	21.625	1.00	37.81
		ATOM	3707	CD	PRO	В	535	-17.529	-9.078	22.640	1.00	38.74
		ATOM	3708	CA	PRO	В	535	-16.608	-7.135	21.492	1.00	36.79
	15	ATOM	3709	CB	PRO	В	535	-17.846	-6.729	22.288	1.00	36.98
		ATOM	3710	CG	PRO	В	535	-18.004	-7.809	23.298	1.00	39.77
		ATOM	3711	C	PRO	В	535	-15.338	-6.494	22.049	1.00	33.95
		MOTA	3712	0	PRO	В	535	-14.786	-6.963	23.040	1.00	34.93
		ATOM	3713	N	LEU	В	536	-14.881	-5.426	21.409	1.00	33.42
	20	ATOM	3714	CA	LEU	В	536	-13.675	-4.732	21.851	1.00	33.40
		ATOM	3715	CB	LEU	В	536	-12.829	-4.314	20.647	1.00	29.31
		ATOM	3716	CG	LEU	В	536	-12.219	-5.433	19.798	1.00	30.06
		ATOM	3717	CD1	LEU	В	536	-11.344	-4.822	18.714	1.00	30.85
		ATOM	3718	CD2	LEU	В	536	-11.398	-6.370	20.676	1.00	28.96
inter.	25	ATOM	3719	C	LEU	В	536	-14.036		22.666	1.00	30.50
		ATOM	3720	0	LEU	В	536	-15.024		22.383	1.00	29.91
163		ATOM	3721	N	TYR	В	537	-13.231		23.676	1.00	28.69
IU		ATOM	3722	CA	TYR	В	537	-13.494		24.505	1.00	29.89
仰		ATOM	3723	CB	TYR	В	537	-12.618		25.750	1.00	32.50
100	30	ATOM	3724	CG	TYR	В	537	-12.849		26.543	1.00	39.46
14.0	50	ATOM	3725	CD1	TYR	В	537	-13.923		27.421	1.00	41.90
- ade		ATOM	3726	CE1	TYR	В	537	-14.174		28.118	1.00	45.72
124		ATOM	3727	CD2	TYR	В	537	-12.022		26.379	1.00	47.39
21		ATOM	3728	CE2	TYR	В	537	-12.262		27.072	1.00	49.93
5.13	35	ATOM	3729	CZ	TYR	В	537	-13.340		27.940	1.00	48.80
1,42	00	ATOM	3730	OH	TYR	В	537	-13.582		28.624	1.00	53.90
1A		ATOM	3731	C	TYR	В	537	-13.262		23.709	1.00	27.09
1010		ATOM	3732	Õ	TYR	В	537	-12.518		22.729	1.00	26.15
157		ATOM	3733	N	ASP	В	538	-13.909		24.141	1.00	26.12
100	40	ATOM	3734	CA	ASP	В	538	-13.830		23.461	1.00	25.27
	70	ATOM	3735	CB	ASP	В	538	-14.748		24.164	1.00	28.85
		ATOM	3736	CG	ASP	В	538	-16.227		23.940	1.00	33.90
		ATOM	3737	OD1	ASP	В	538	-17.052		24.819	1.00	32.68
		ATOM	3738	OD2	ASP	В	538	-16.562		22.882	1.00	38.26
	45	ATOM	3739	C	ASP	В	538	-12.447		23.261	1.00	25.18
	7.5	ATOM	3740	0	ASP	В	538	-12.120		22.147	1.00	26.41
		ATOM	3741	N	LEU	В	539	-11.637		24.313	1.00	20.76
		ATOM	3742	CA	LEU	В	539	-10.312		24.150	1.00	19.65
		ATOM	3742	CB	LEU	В	539	-9.567		25.496	1.00	17.48
	50	ATOM	3744	CG	LEU	В	539	-8.116		25.469	1.00	16.46
	50	ATOM	3745	CD1	LEU	В	539	-8.051		24.838	1.00	16.43
				CD2	LEU	В	539	-7.564		26.895	1.00	15.57
		ATOM	3746					-9.484		23.127	1.00	16.75
		ATOM	3747	C	LEU	В	539	-8.862		22.249	1.00	20.36
	==	ATOM	3748	0	LEU	В	539			23.239		18.23
	55	ATOM	3749	N	LEU	В	540	-9.487			1.00	
		MOTA	3750	CA	LEU	В	540	-8.743		22.319	1.00	18.05
		ATOM	3751	CB	LEU	В	540	-8.909		22.701	1.00	16.38
		MOTA	3752	CG	LEU	В	540	-8.188		21.821	1.00	19.81
	60	MOTA	3753	CD1	LEU	В	540	-6.679		21.828	1.00	19.27
	60	MOTA	3754	CD2	LEU	В	540	-8.473		22.327	1.00	18.00
		ATOM	3755	C	LEU	В	540	-9.241		20.891	1.00	21.50
		ATOM	3756	0	LEU	В	540	-8.449	0.293	19.964	1.00	20.41

	5	ATOM	3757	N	LEU	В	541	-10.559	0.206 20.726	1.00	22.40
		ATOM	3758	CA	LEU	В	541	-11.164	0.419 19.413	1.00	23.27
		ATOM	3759	CB	LEU	В	541	-12.686	0.429 19.527	1.00	25.12
		ATOM	3760	CG	LEU	В	541	-13.410	-0.808 18.999	1.00	36.53
		ATOM	3761	CD1	LEU	В	541	-14.910	-0.671 19.273	1.00	30.98
	10	ATOM	3762	CD2	LEU	В	541	-13.136	-0.971 17.508	1.00	31.93
	10										
		ATOM	3763	C	LEU	В	541	-10.697	1.751 18.842	1.00	22.46
		ATOM	3764	0	LEU	В	541	-10.359	1.845 17.666	1.00	26.29
		ATOM	3765	N	GLU	В	542	-10.694	2.781 19.680	1.00	23.96
		ATOM	3766	CA	GLU	В	542	-10.248	4.106 19.270	1.00	26.91
	15	MOTA	3767	CB	GLU	В	542	-10.250	5.050 20.468	1.00	30.84
		MOTA	3768	CG	GLU	В	542	-11.166	6.245 20.347	1.00	37.20
		MOTA	3769	CD	GLU	В	542	-11.138	7.105 21.597	1.00	39.98
		ATOM	3770	OE1	GLU	В	542	-12.223	7.385 22.144	1.00	39.92
		ATOM	3771	OE2	GLU	В	542	-10.028	7.494 22.034	1.00	38.96
	20	ATOM	3772	C	GLU	В	542	-8.826	4.010 18.724	1.00	27.90
		ATOM	3773	0	GLU	В	542	-8.530	4.492 17.634	1.00	29.32
		ATOM	3774	N	MET	В	543	-7.945	3.388 19.499	1.00	26.41
		ATOM	3775	CA	MET	В	543	-6.552	3.237 19.107	1.00	23.53
		ATOM	3776	CB	MET	В	543	-5.749	2.591 20.247	1.00	24.60
	25	ATOM	3777	CG	MET	В	543	-5.812	3.338 21.579	1.00	26.46
13	23	ATOM	3778	SD	MET	В	543	-5.373	5.084 21.467	1.00	29.45
:22			3779	CE	MET	В	543	-3.585	4.971 21.349		25.43
19.1		MOTA								1.00	
(4)		MOTA	3780	C	MET	В	543	-6.403	2.407 17.832	1.00	25.80
1,50	20	ATOM	3781	0	MET	В	543	-5.535	2.686 17.004	1.00	23.59
74.3	30	ATOM	3782	N	LEU	В	544	-7.254	1.394 17.673	1.00	27.74
į.a.		ATOM	3783	CA	LEU	В	544	-7.202	0.522 16.499	1.00	26.32
343		ATOM	3784	CB	LEU	В	544	-8.069	-0.721 16.719	1.00	26.75
31		MOTA	3785	CG	LEU	В	544	-8.274	-1.632 15.502	1.00	28.12
1774		MOTA	3786	CD1	LEU	В	544	-6.956	-2.294 15.136	1.00	26.36
E LOS	35	ATOM	3787	CD2	LEU	В	544	-9.330	-2.680 15.803	1.00	27.00
2.1		MOTA	3788	C	LEU	В	544	-7.672	1.252 15.250	1.00	26.97
11		ATOM	3789	0	LEU	В	544	-7.036	1.181 14.195	1.00	24.25
75.0		MOTA	3790	N	ASP	В	545	-8.787	1.961 15.372	1.00	30.37
10		MOTA	3791	CA	ASP	В	545	-9.338	2.702 14.244	1.00	32.34
+0	40	MOTA	3792	CB	ASP	В	545	-10.668	3.346 14.637	1.00	36.61
		ATOM	3793	CG	ASP	В	545	-11.818	2.370 14.565	1.00	42.73
		ATOM	3794	OD1	ASP	В	545	-12.858	2.624 15.211	1.00	47.39
		ATOM	3795	OD2	ASP	В	545	-11.676	1.342 13.863	1.00	46.96
		ATOM	3796	C	ASP	В	545	-8.382	3.762 13.711	1.00	31.27
	45	ATOM	3797	0	ASP	В	545	-8.443	4.120 12.532	1.00	30.53
	73	ATOM	3798	N	ALA	В	546	-7.506	4.272 14.572	1.00	29.02
		ATOM	3799	CA	ALA	В	546	-6.543	5.280 14.141	1.00	31.21
				CB	ALA	В		-5.646	5.693 15.306	1.00	30.98
		ATOM	3800				546				
	50	ATOM	3801	C	ALA	В	546	-5.697	4.731 12.996	1.00	32.14
	50	ATOM	3802	0	ALA	В	546	-5.189	5.490 12.170	1.00	33.78
		ATOM	3803	N	HIS	В	547	-5.555	3.410 12.943	1.00	32.27
		MOTA	3804	CA	HIS	В	547	-4.773	2.767 11.892	1.00	37.73
		MOTA	3805	CB	HIS	В	547	-3.991	1.576 12.457	1.00	35.83
		MOTA	3806	CG	HIS	В	547	-2.796	1.968 13.269	1.00	34.54
	55	ATOM	3807	CD2	HIS	В	547	-2.698	2.553 14.486	1.00	30.23
		ATOM	3808	ND1	HIS	В	547	-1.502	1.755 12.840	1.00	34.23
		ATOM	3809	CE1	HIS	В	547	-0.659	2.193 13.760	1.00	36.72
		ATOM	3810	NE2	HIS	В	547	-1.360	2.681 14.768	1.00	31.48
		ATOM	3811	C	HIS	В	547	-5.649	2.286 10.735	1.00	43.69
	60	ATOM	3812	ō	HIS	В	547	-5.178	2.152 9.606	1.00	46.04
		ATOM	3813	N	ARG	В	548	-6.919	2.020 11.019	1.00	48.35
		ATOM	3814	CA	ARG	В	548	-7.843	1.551 9.993	1.00	54.74
		-11 011	5524	0		_					

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	5	MOTA	3815	CB	ARG	В	548	-8.522	0.267	10.452	1.00	54.66
		ATOM	3816	C	ARG	В	548	-8.886	2.619	9.681	1.00	59.94
		MOTA	3817	0	ARG	В	548	-8.580	3.812	9.672	1.00	62.81
		ATOM	3818	N	LEU	В	549	-10.116	2.186	9.422	1.00	64.81
		MOTA	3819	CA	LEU	В	549	-11.204	3.109	9.112	1.00	67.59
	10	MOTA	3820	CB	LEU	В	549	-12.478	2.327	8.799	1.00	68.06
		MOTA	3821	C	LEU	В	549	-11.449	4.069	10.275	1.00	69.12
		MOTA	3822	0	LEU	В	549	-11.451	5.297	10.036	1.00	68.96
		MOTA	3823	OXT	LEU	В	549	-11.634	3.579	11.412	1.00	70.70
		HETATM	3824	CP9	DES	В	600	-4.547	-6.077	22.000	1.00	18.55
	15	HETATM	3825	CP8	DES	В	600	-3.163	-6.365	21.467	1.00	17.72
		HETATM	3826	CP7	DES	В	600	-2.897	-7.853	21.381	1.00	21.17
		HETATM	3827	CP6	DES	В	600	-3.719	-8.551	20.374	1.00	22.05
		HETATM	3828	CP1	DES	В	600	-3.405	-8.481	18.998	1.00	21.32
		HETATM	3829	CP2	DES	В	600	-4.239	-9.095	18.063	1.00	21.61
	20	HETATM	3830	CP3	DES	В	600	-5.388	-9.771	18.509	1.00	24.89
		HETATM	3831	OP3	DES	В	600	-6.244	-10.339	17.600	1.00	24.94
		HETATM	3832	CP4	DES	В	600	-5.718	-9.858	19.860	1.00	24.08
		HETATM	3833	CP5	DES	В	600	-4.877	-9.240	20.791	1.00	24.67
		HETATM	3834	C7	DES	В	600	-1.998	-8.460		1.00	16.67
4770	25	HETATM	3835	C6	DES	В	600	-1.330	-7.834		1.00	15.39
		HETATM	3836	C5	DES	В	600	-2.054	-7.642		1.00	17.62
365		HETATM	3837	C4	DES	В	600	-1.433	-7.072		1.00	16.16
113		HETATM	3838	C3	DES	В	600	-0.077	-6.685		1.00	20.04
27.0		HETATM	3839	03	DES	В	600	0.509	-6.113		1.00	15.55
gray.	30	HETATM	3840	C2	DES	В	600	0.669	-6.866		1.00	18.94
14		HETATM	3841	C1	DES	В	600	0.035	-7.440		1.00	15.20
g. in		HETATM	3842	C8	DES	В	600	-1.642	-9.903		1.00	17.61
3.4		HETATM	3843	C9	DES	В	600	-0.440	-10.009		1.00	11.63
#1		HETATM	3844	C1	CBM	В	417	-4.997	-22.994		1.00	55.80
(10)	35	HETATM	3845	04	CBM	В	417	-4.789	-24.187		1.00	55.56
لدا		HETATM	3846	03	CBM	В	417	-4.798	-22.559		1.00	56.04
L.		HETATM	3847	C2	CBM	В	417	-5.468	-21.960		1.00	57.04
122		HETATM	3848	C1	CBM	В	530	-15.278	-5.124		1.00	87.39
+0		HETATM	3849	04	CBM	В	530	-15.852	-5.086	9.064	1.00	87.68
400	40	HETATM	3850	03	CBM	В	530	-15.832	-4.291		1.00	86.22
		HETATM	3851	C2	CBM	В	530	-14.207	-5.886		1.00	87.65
		ATOM	3852	CB	HIS	C	687	9.818	-20.030		1.00	63.34
		ATOM	3853	C	HIS	C	687	10.133	-20.267		1.00	63.49
		ATOM	3854	0	HIS	c	687		-20.840		1.00	63.87
	45	ATOM	3855	N	HIS	Č	687		-19.563		1.00	65.42
		ATOM	3856	CA	HIS	c	687	9.424	-19.484		1.00	64.86
		ATOM	3857	N	LYS	c	688	9.533	-20.281		1.00	62.00
		ATOM	3858	CA	LYS	C	688	10.101	-20.999		1.00	60.81
		ATOM	3859	CB	LYS	C	688	8.980	-21.540		1.00	61.76
	50	ATOM	3860	CD	LYS	C	688	11.050	-20.127		1.00	57.47
	50	ATOM	3861	0	LYS	c	688	12.253	-20.127		1.00	57.64
		ATOM	3862	N	ILE	C	689	10.511	-19.103		1.00	55.74
		ATOM	3863	CA	ILE	C	689	11.326	-18.212			
											1.00	53.09
	55	ATOM ATOM	3864 3865	CB CG2	ILE	C	689 689	10.496 11.334	-17.057 -16.286-		1.00	53.83
	55										1.00	54.55
		MOTA MOTA	3866	CG1 CD1	ILE	C	689		-17.603-		1.00	52.90
			3867		ILE	С	689		-16.550-		1.00	50.45
		MOTA	3868	C	ILE	С	689	12.513	-17.611		1.00	50.82
	60	ATOM	3869	O N	ILE	C	689		-17.550		1.00	51.28
	00	ATOM	3870		LEU	C	690		-17.162		1.00	48.01
		ATOM	3871	CA	LEU	C	690		-16.570		1.00	47.33
		MOTA	3872	CB	LEU	С	690	12.812	-16.058	-5.199	1.00	42.51

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	5	MOTA	3873	CG	LEU	C	690	13.835 -15.501 -4.206 1.00 40.67
		ATOM	3874		LEU	C	690	14.575 -14.324 -4.831 1.00 39.95
		MOTA	3875	CD2	LEU	C	690	13.128 ~15.078 -2.926 1.00 38.77
		ATOM	3876	C	LEU	C	690	14.445 -17.615 -6.282 1.00 48.87
		ATOM	3877	0	LEU	C	690	15.643 -17.340 -6.393 1.00 46.71
	10	ATOM	3878	N	HIS	C	691	14.001 -18.818 -5.939 1.00 51.36
		ATOM	3879	CA	HIS	C	691	14.886 -19.946 -5.675 1.00 53.35
		ATOM	3880	CB	HIS	Ċ	691	14.042 -21.203 -5.460 1.00 58.64
		ATOM	3881	CG	HIS	C	691	14.655 -22.195 -4.526 1.00 62.94
		ATOM	3882	CD2	HIS	Ċ	691	15.503 -23.227 -4.751 1.00 64.95
	15	ATOM	3883	ND1	HIS	C	691	14.392 -22.202 -3.173 1.00 65.49
	13	ATOM	3884	CE1	HIS	C	691	
		ATOM	3885	NE2	HIS	C	691	
		ATOM	3886	C	HIS			15.733 -23.833 -3.540 1.00 68.77
						C	691	15.824 -20.162 -6.861 1.00 52.19
	20	ATOM	3887	0	HIS	C	691	17.048 -20.153 -6.717 1.00 47.53
	20	ATOM	3888	N	ARG	C	692	15.222 -20.350 -8.032 1.00 52.37
		ATOM	3889	CA	ARG	C	692	15.949 -20.586 -9.271 1.00 52.90
		ATOM	3890	CB	ARG	C	692	14.955 -20.832-10.410 1.00 54.04
		MOTA	3891	CG	ARG	C	692	15.575 -20.826-11.797 1.00 57.52
		ATOM	3892	CD	ARG	C	692	14.528 -21.048-12.874 1.00 58.25
(2)	25	ATOM	3893	NE	ARG	C	692	14.375 -19.878-13.732 1.00 61.43
10		MOTA	3894	CZ	ARG	C	692	13.218 -19.260-13.951 1.00 64.32
n.		ATOM	3895	NH1	ARG	C	692	12.108 -19.706-13.378 1.00 63.22
		ATOM	3896	NH2	ARG	C	692	13.171 -18.197-14.746 1.00 65.93
(10)		ATOM	3897	C	ARG	C	692	16.873 -19.434 -9.639 1.00 53.09
(al	30	ATOM	3898	0	ARG	C	692	18.047 -19.644 -9.956 1.00 53.06
1		ATOM	3899	N	LEU	C	693	16.338 -18.217 -9.607 1.00 50.73
lest:		ATOM	3900	CA	LEU	C	693	17.125 -17.039 -9.945 1.00 49.53
14		ATOM	3901	CB	LEU	C	693	16.249 -15.784 -9.881 1.00 49.56
91		ATOM	3902	CG	LEU	C	693	15.781 -15.245-11.239 1.00 49.78
1	35	ATOM	3903	CD1	LEU	C	693	15.219 -16.389-12.079 1.00 50.30
لنا		ATOM	3904	CD2	LEU	Č	693	14.728 -14.170-11.037 1.00 48.79
W		ATOM	3905	C	LEU	C	693	18.318 -16.904 -9.006 1.00 48.38
255		ATOM	3906	0	LEU	C	693	19.382 -16.426 -9.402 1.00 46.35
40		ATOM	3907	N	LEU	C	694	18.135 -17.329 -7.761 1.00 46.74
Ø	40	ATOM	3908	CA	LEU	c	694	19.204 -17.272 -6.775 1.00 49.41
		ATOM	3909	CB	LEU	c	694	18.634 -17.415 -5.362 1.00 45.20
		ATOM	3910	CG	LEU	C	694	18.222 -16.128 -4.643 1.00 40.19
		ATOM	3911	CD1	LEU	C	694	17.456 -16.474 -3.371 1.00 41.65
		ATOM	3912	CD2	LEU	C	694	19.453 -15.307 -4.317 1.00 35.91
	45	ATOM	3913	C	LEU	C	694	
	13	ATOM	3914	0	LEU	C	694	
								21.370 -18.320 -6.776 1.00 53.55
		ATOM	3915	N	GLN	C	695	19.634 -19.498 -7.619 1.00 57.44
		ATOM	3916	CA	GLN	C	695	20.416 -20.685 -7.959 1.00 62.46
	50	ATOM	3917	CB	GLN	C	695	19.477 -21.853 -8.304 1.00 61.95
	50	ATOM	3918	CG	GLN	C	695	19.548 -23.010 -7.311 1.00 61.49
		ATOM	3919	CD	GLN	C	695	18.454 -24.053 -7.490 1.00 62.78
		MOTA	3920	OE1	GLN	C	695	18.262 -24.928 -6.653 1.00 63.33
		ATOM	3921	NE2	GLN	C	695	17.720 -23.969 -8.608 1.00 60.37
		MOTA	3922	C	GLN	C	695	21.330 -20.414 -9.149 1.00 65.13
	55	MOTA	3923	0	GLN	C	695	22.517 -20.740 -9.116 1.00 65.87
		ATOM	3924	N	ASP	C	696	20.761 -19.824-10.197 1.00 67.67
		ATOM	3925	CA	ASP	C	696	21.492 -19.500-11.420 1.00 70.66
		MOTA	3926	CB	ASP	C	696	20.801 -18.348-12.151 1.00 71.06
		MOTA	3927	CG	ASP	C	696	20.127 -18.792-13.430 1.00 71.70
	60	MOTA	3928	OD1	ASP	C	696	20.637 -18.455-14.521 1.00 72.47
		ATOM	3929	OD2	ASP	C	696	19.086 -19.478-13.342 1.00 71.41
		ATOM	3930	C	ASP	Ĉ	696	22.951 -19.132-11.169 1.00 72.41

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	5	ATOM	3931	0	ASP	C	696	23.245	-18.115-10.541	1.00	72.56
		ATOM	3932	N	SER	C	697	23.859	-19.967-11.668	1.00	74.67
		ATOM	3933	CA	SER	C	697	25.291	-19.741-11.507	1.00	76.45
		ATOM	3934	CB	SER	C	697	26.019	-21.076-11.377	1.00	76.00
		ATOM	3935	C	SER	C	697	25.841	-18.960-12.696	1.00	78.44
	10	ATOM	3936	0	SER	C	697	26.286	-17.809-12.489	1.00	79.20
		ATOM	3937	OXT	SER	C	697	25.818	-19.510-13.820	1.00	80.07
		ATOM	3938	CB	LYS	D	686	-14.070	13.661 16.843	1.00	50.28
		ATOM	3939	c	LYS	D	686	-13.682	14.418 19.199	1.00	51.59
		ATOM	3940	ō	LYS	D	686	-12.629	14.738 19.759	1.00	50.42
	15	ATOM	3941	N	LYS	D	686	-12.029	15.796 17.283	1.00	
	10	ATOM	3942	CA	LYS	D	686				50.43
		ATOM	3943	N	HIS			-13.976	14.872 17.769	1.00	50.62
		ATOM	3944	CA		D	687	-14.617	13.676 19.787	1.00	49.91
					HIS	D	687	-14.447	13.176 21.144	1.00	51.28
	20	ATOM	3945	CB	HIS	D	687	-15.806	12.984 21.828	1.00	54.12
	20	ATOM	3946	CG	HIS	D	687	-15.713	12.336 23.177	1.00	60.06
		ATOM	3947	CD2	HIS	D	687	-15.418	11.064 23.539	1.00	61.05
		ATOM	3948	ND1	HIS	D	687	-15.911	13.030 24.352	1.00	62.39
		ATOM	3949	CE1	HIS	D	687	-15.741	12.215 25.378	1.00	62.76
		ATOM	3950	NE2	HIS	D	687	-15.441	11.016 24.912	1.00	63.46
122	25	ATOM	3951	C	HIS	D	687	-13.691	11.849 21.163	1.00	49.55
		ATOM	3952	0	HIS	D	687	-14.099	10.878 20.524	1.00	50.84
E		ATOM	3953	N	LYS	D	688	-12.593	11.816 21.909	1.00	44.00
10		ATOM	3954	CA	LYS	D	688	-11.784	10.611 22.038	1.00	40.31
esta esta		ATOM	3955	CB	LYS	D	688	-10.446	10.773 21.299	1.00	41.42
	30	ATOM	3956	CG	LYS	D	688	-10.513	10.595 19.780	1.00	42.76
74.5		ATOM	3957	CD	LYS	D	688	-9.123	10.716 19.152	1.00	38.66
i di		MOTA	3958	CE	LYS	D	688	-9.162	10.529 17.640	1.00	38.28
100		ATOM	3959	NZ	LYS	D	688	-7.894	10.970 16.986	1.00	31.58
11		ATOM	3960	C	LYS	D	688	-11.506	10.378 23.517	1.00	36.70
	35	MOTA	3961	0	LYS	D	688	-11.271	11.326 24.266	1.00	33.38
1,U		ATOM	3962	N	ILE	D	689	-11.549	9.122 23.942	1.00	33.06
1,0		ATOM	3963	CA	ILE	D	689	-11.255	8.806 25.328	1.00	28.70
100		ATOM	3964	CB	ILE	D	689	-11.438	7.301 25.607	1.00	30.88
10		ATOM	3965	CG2	ILE	D	689	-10.725	6.912 26.899	1.00	31.45
1	40	ATOM	3966	CG1	ILE	D	689	-12.927	6.971 25.721	1.00	32.57
		ATOM	3967	CD1	ILE	D	689	-13.308	5.679 25.031	1.00	29.79
		ATOM	3968	C	ILE	D	689	-9.790	9.193 25.541	1.00	27.64
		ATOM	3969	ō	ILE	D	689	-9.405	9.649 26.611	1.00	25.54
		ATOM	3970	N	LEU	D	690	-8.985	9.021 24.496	1.00	24.25
	45	ATOM	3971	CA	LEU	D	690	-7.563	9.348 24.549	1.00	26.63
		ATOM	3972	CB	LEU	D	690	-6.903	9.021 23.200	1.00	22.83
		ATOM	3973	CG	LEU	D	690	-5.433	9.387 22.992	1.00	25.47
		ATOM	3974	CD1	LEU	D	690	-4.595	8.772 24.108	1.00	24.03
		ATOM	3975	CD2	LEU	D	690	-4.956	8.898 21.616	1.00	
	50	ATOM	3976	C	LEU	D	690				20.87
	50	ATOM	3977		LEU	D		-7.344	10.823 24.902	1.00	26.64
		ATOM	3977	N	HIS	D	690	-6.408	11.165 25.625	1.00	28.34
		ATOM					691	-8.206	11.694 24.383	1.00	27.77
			3979	CA	HIS	D	691	-8.107	13.125 24.665	1.00	29.16
	55	ATOM	3980	CB	HIS	D	691	-9.156	13.907 23.861	1.00	30.89
	33	ATOM	3981	CG	HIS	D	691	-8.903	13.935 22.386	1.00	37.09
		ATOM	3982	CD2	HIS	D	691	-7.750	14.000 21.679	1.00	41.39
		ATOM	3983	ND1	HIS	D	691	-9.920	13.906 21.458	1.00	41.65
		ATOM	3984	CE1	HIS	D	691	-9.407	13.953 20.242	1.00	44.64
		ATOM	3985	NE2	HIS	D	691	-8.091	14.010 20.347	1.00	41.94
	60	ATOM	3986	C	HIS	D	691	-8.338	13.373 26.159	1.00	26.65
		ATOM	3987	0	HIS	D	691	-7.602	14.120 26.802	1.00	24.50
		ATOM	3988	N	ARG	D	692	-9.371	12.742 26.703	1.00	25.70

	5	ATOM	3989	CA	ARG	D	692	-9.691	12.912 28.114	1.00	29.11
		ATOM	3990	CB	ARG	D	692	-10.959	12.134 28.472	1.00	30.84
		ATOM	3991	CG	ARG	D	692	-11.255	12.129 29.963	1.00	41.63
		ATOM	3992	CD	ARG	D	692	-12.502	11.327 30.290	1.00	48.83
		ATOM	3993	NE	ARG	D	692	-13.618	12.198 30.647	1.00	54.50
	10	ATOM	3994	CZ							
	10				ARG	D	692	-14.498	12.677 29.774	1.00	59.37
		ATOM	3995	NH1	ARG	D	692	-14.392	12.371 28.486	1.00	60.97
		ATOM	3996	NH2	ARG	D	692	-15.483	13.464 30.188	1.00	59.07
		ATOM	3997	C	ARG	D	692	-8.548	12.451 29.011	1.00	28.30
		MOTA	3998	0	ARG	D	692	-8.139	13.167 29.929	1.00	26.50
	15	MOTA	3999	N	LEU	D	693	-8.030	11.259 28.737	1.00	24.87
		MOTA	4000	CA	LEU	D	693	-6.943	10.705 29.536	1.00	27.17
		ATOM	4001	CB	LEU	D	693	-6.674	9.254 29.116	1.00	28.45
		ATOM	4002	CG	LEU	D	693	-7.844	8.300 29.391	1.00	30.40
		ATOM	4003	CD1	LEU	D	693	-7.575	6.932 28.778	1.00	34.79
	20	ATOM	4004	CD2	LEU	D	693	-8.043	8.171 30.894		
	20									1.00	32.02
		ATOM	4005	C	LEU	D	693	-5.670	11.539 29.440	1.00	25.96
		ATOM	4006	0	LEU	D	693	-4.948	11.700 30.428	1.00	27.01
		ATOM	4007	N	LEU	D	694	-5.395	12.080 28.257	1.00	25.33
	~ "	ATOM	4008	CA	LEU	D	694	-4.207	12.906 28.062	1.00	27.22
inc	25	ATOM	4009	CB	LEU	D	694	-3.948	13.126 26.572	1.00	24.61
(3)		MOTA	4010	CG	LEU	D	694	-3.118	12.080 25.825	1.00	22.20
:0		MOTA	4011	CD1	LEU	D	694	-3.230	12.332 24.324	1.00	21.13
ru:		ATOM	4012	CD2	LEU	D	694	-1.666	12.148 26.275	1.00	21.34
(.0)		ATOM	4013	C	LEU	D	694	-4.336	14.270 28.742	1.00	32.40
į "i	30	ATOM	4014	0	LEU	D	694	-3.339	14.889 29.102	1.00	31.55
4.4		ATOM	4015	N	GLN	D	695	-5.570	14.733 28.915	1.00	36.93
i mai		ATOM	4016	CA	GLN	D	695	-5.820	16.032 29.528	1.00	43.18
1.		ATOM	4017	CB	GLN	D	695	-7.022			
41									16.694 28.862	1.00	40.48
100	35	ATOM	4018	CG	GLN	D	695	-6.772	17.071 27.422	1.00	37.99
Į.J	33	ATOM	4019	CD	GLN	D	695	-7.943	17.764 26.795	1.00	35.86
2.1		ATOM	4020	OE1	GLN	D	695	-7.863	18.895 26.342	1.00	38.84
		ATOM	4021	NE2	GLN	D	695	-9.082	17.060 26.757	1.00	31.62
Aser		MOTA	4022	C	GLN	D	695	-6.049	16.009 31.034	1.00	48.74
443		ATOM	4023	0	GLN	D	695	-6.119	17.065 31.660	1.00	51.25
157	40	ATOM	4024	N	ASP	D	696	-6.175	14.818 31.611	1.00	54.01
		ATOM	4025	CA	ASP	D	696	-6.398	14.702 33.047	1.00	62.23
		MOTA	4026	CB	ASP	D	696	-6.217	13.238 33.485	1.00	63.97
		ATOM	4027	CG	ASP	D	696	-7.527	12.467 33.475	1.00	67.72
		ATOM	4028	OD1	ASP	D	696	-8.528	12.996 32.941	1.00	68.11
	45	ATOM	4029	OD2	ASP	D	696	-7.552	11.333 34.003	1.00	68.95
		ATOM	4030	C	ASP	D	696	-5.456	15.622 33.840		
		ATOM	4031	0	ASP	D	696	-4.312		1.00	65.60
									15.189 34.134	1.00	68.33
		ATOM	4032	OXT	ASP	D	696	-5.874	16.755 34.140	1.00	69.20
		HETATM	4033	0	HOH		1	16.153	-0.605 -4.425	1.00	17.11
	50	HETATM	4034	0	HOH		2	16.570	-5.304-16.560	1.00	21.44
		HETATM	4035	0	HOH		3	18.526	0.742 -4.495	1.00	23.43
		HETATM	4036	0	HOH		4	13.647	-2.187 8.588	1.00	25.82
		HETATM	4037	0	HOH		5	9.778	-5.825 2.509	1.00	20.58
		HETATM	4038	0	HOH		6	17.072	-3.605 -8.015	1.00	18.38
	55	HETATM	4039	ō	HOH		7	24.920	-1.689 -2.780	1.00	25.74
		HETATM	4040	ō	НОН		8	7.321	-5.649 5.061	1.00	24.11
		HETATM	4041	o	HOH		9	25.976	-3.535 15.158	1.00	26.78
		HETATM	4041	0	HOH		10	15.088			
									-7.006-15.192	1.00	19.64
	60	HETATM	4043	0	HOH		11	14.070	0.925 -5.953	1.00	20.55
	00	HETATM	4044	0	HOH		12	18.008	3.407 -6.654	1.00	32.30
		HETATM	4045	0	HOH		13	31.949	-8.393 13.487	1.00	30.64
		HETATM	4046	0	HOH		14	19.625	-2.804 -4.279	1.00	24.45

	5	HETATM	4047	0	HOH	15	11.741	1.079-21.140	1.00	25.87
		HETATM	4048	0	HOH	16	25.067	13.951 14.153	1.00	31.07
		HETATM	4049	0	HOH	17	15.501	1.323-10.393	1.00	21.01
		HETATM	4050	0	HOH	18	13.880	3.349-11.482	1.00	24.28
		HETATM	4051		HOH	19	17.591	0.979 -8.828	1.00	35.26
	10	HETATM	4052		HOH	20	23.682	-2.041 -0.314	1.00	37.90
		HETATM	4053	0						
					HOH	21	15.754	9.496 11.841	1.00	39.44
		HETATM	4054	0	нон	22	-4.943	7.574 -3.066	1.00	37.67
		HETATM	4055	0	нон	23	6.877	0.354-15.982	1.00	36.92
	1.5	HETATM	4056	0	HOH	24	15.806	-4.002 8.671	1.00	30.38
	15	HETATM	4057		HOH	25	17.185	-3.158 -5.321	1.00	28.89
		HETATM	4058	0	HOH	26	17.572	9.249 17.009	1.00	30.15
		HETATM	4059	0	HOH	27	24.096	-2.929 11.604	1.00	31.37
		HETATM	4060	0	HOH	28	22.324	-5.871-11.980	1.00	32.74
		HETATM	4061	0	HOH	29	27.547	-12.361 -0.801	1.00	36.61
	20	HETATM	4062	0	HOH	30	11.173	13.442 -2.719	1.00	35.41
		HETATM	4063	0	HOH	31	15.438	-9.527 5.483	1.00	29.88
		HETATM	4064	ō	нон	32	9.946	-6.564 5.983	1.00	35.05
		HETATM	4065	o	HOH	33	7.599	11.680-15.261	1.00	38.68
		HETATM	4066	ō	нон	34	20.112	10.503 -5.109	1.00	42.66
	25	HETATM	4067	0	HOH					
180	23					35	15.972	10.343 14.897	1.00	41.73
153		HETATM	4068	0	HOH	36	22.401	-5.914 -9.527	1.00	28.08
11.		HETATM	4069	0	нон	37	16.128	-0.899 -8.109	1.00	33.13
(0		HETATM	4070	0	HOH	38	3.581	15.655 -3.706	1.00	41.37
1.4		HETATM	4071	0	HOH	39	31.900	13.545 21.339	1.00	37.79
A	30	HETATM	4072	0	HOH	40	20.058	-7.530 14.119	1.00	47.51
i rada		HETATM	4073	0	HOH	41	34.634	6.668 15.632	1.00	29.24
had		HETATM	4074	0	HOH	42	17.968	10.511 -9.085	1.00	44.60
		HETATM	4075	0	HOH	43	23.258	-17.325 -4.088	1.00	44.10
25		HETATM	4076	0	HOH	44	4.034	-1.472 27.521	1.00	15.22
	35	HETATM	4077	0	HOH	45	-5.943	-0.018 36.088	1.00	21.11
£.J		HETATM	4078	0	HOH	46	6.084	-1.509 29.478	1.00	19.51
14		HETATM	4079	0	HOH	47	9.762	1.061 15.621	1.00	27.74
		HETATM	4080	0	нон	48	1.804	0.717 17.260	1.00	20.97
123		HETATM	4081	0	HOH	49	0.929	0.421 30.281	1.00	19.64
10	40	HETATM	4082	ō	нон	50	9.627	4.271 31.231	1.00	19.02
		HETATM	4083	ō	HOH	51	2.121	-0.261 13.654	1.00	26.09
		HETATM	4084	0	нон	52	20.060	10.275 17.711		
		HETATM	4085	0	нон	53			1.00	25.49
		HETATM	4086				-6.786	0.736 33.483	1.00	22.34
	45			0	нон	54	2.751	-4.136 27.760	1.00	19.93
	43	HETATM	4087	0	нон	55	5.994	-4.079 31.292	1.00	32.27
		HETATM	4088	0	HOH	56	19.416	16.921 21.645	1.00	25.54
		HETATM	4089	0	HOH	57	4.833	2.325 29.006	1.00	19.00
		HETATM	4090	0	HOH	58	-7.638	-8.931 37.809	1.00	24.79
		HETATM	4091	0	HOH	59	28.442	-4.673 21.875	1.00	24.32
	50	HETATM	4092	0	HOH	60	1.094	-4.893 32.100	1.00	24.27
		HETATM	4093	0	HOH	61	0.905	-7.306 32.783	1.00	21.33
		HETATM	4094	0	HOH	62	3.396	-2.971 32.306	1.00	26.13
		HETATM	4095	0	HOH	63	10.363	4.576 28.391	1.00	33.43
		HETATM	4096	0	HOH	64	19.551	-6.473 16.597	1.00	35.38
	55	HETATM	4097	ō	HOH	65	-2.888	-19.627 15.665	1.00	27.99
		HETATM	4098	ō	нон	66	-7.275	-9.745 31.077	1.00	27.00
		HETATM	4099	0	HOH	67	10.189	3.580 16.510	1.00	24.19
		HETATM	4100	0	HOH	68				
							2.741	0.716 28.382	1.00	16.48
	60	HETATM HETATM	4101	0	HOH	69	23.522	-4.323 13.943	1.00	27.48
	50		4102	0	HOH	70	17.133	8.133 19.686	1.00	32.24
		HETATM	4103	0	HOH	71	-0.295	4.535 35.884	1.00	33.42
		HETATM	4104	0	HOH	72	9.519	10.828 34.842	1.00	29.38

	5	HETATM	4105	0	HOH	73	6.291	14.878 29.070	1.00	28.21
		HETATM	4106	0	HOH	74	-1.721	6.480 13.381	1.00	49.91
		HETATM	4107	0	HOH	75	10.091	-15.427 26.194	1.00	24.17
		HETATM	4108	0	HOH	76	5.029	7.461 17.718	1.00	18.91
		HETATM	4109	0	HOH	77	3.758	2.086 14.306	1.00	28.28
	10	HETATM	4110	ō	нон	78	-1.390	-18.739 33.183	1.00	41.11
		HETATM	4111	ō	нон	79	12.703	-8.687 32.119	1.00	36.21
		HETATM	4112	0	нон	80	22.270	-6.451 14.844	1.00	33.21
		HETATM	4113	0	нон	81				
							1.458	4.605 34.026	1.00	23.59
	15	HETATM	4114	0	нон	82	1.759	-2.158 30.374	1.00	28.78
	13	HETATM	4115	0	нон	83	6.153	-21.372 23.188	1.00	31.14
		HETATM	4116	0	нон	84	36.525	0.463 20.792	1.00	45.26
		HETATM	4117	0	HOH	85	13.832	9.696 13.792	1.00	33.12
		HETATM	4118	0	HOH	86	31.166	6.635 24.924	1.00	35.19
		HETATM	4119	0	HOH	87	8.844	-10.389 34.180	1.00	48.80
	20	HETATM	4120	0	HOH	88	9.581	-6.956 34.136	1.00	42.95
		HETATM	4121	0	HOH	89	-1.563	15.887 27.596	1.00	39.35
		HETATM	4122	0	HOH	90	-5.286	10.345 32.757	1.00	35.20
		HETATM	4123	0	HOH	91	15.035	0.607 13.339	1.00	29.53
		HETATM	4124	0	HOH	92	-10.984	-1.500 30.272	1.00	29.84
11.770	25	HETATM	4125	0	нон	93	-7.239	-0.271 -1.207	1.00	48.98
		HETATM	4126	ō	нон	94	18.022	-4.902 34.286	1.00	35.28
		HETATM	4127	ō	нон	95	29.347	-6.319 19.920	1.00	37.20
112		HETATM	4128	o	нон	96	-14.309	-19.369 20.945	1.00	30.23
10		HETATM	4129	0	нон	97	31.496	4.614 18.716	1.00	38.79
Louis	30	HETATM	4130	Ö	нон	98	26.567	9.759 25.629	1.00	
1	50	HETATM	4131	0	HOH	99				29.72
Sech				0			2.848	14.531 1.134	1.00	38.08
1/4		HETATM	4132		нон	100	-9.373	5.699 -7.953	1.00	53.23
Ð		HETATM	4133	0	HOH	101	-10.137	-0.553 -6.742	1.00	47.72
(.)	2.5	HETATM	4134	0	HOH	102	10.558	-10.363 15.403	1.00	40.97
1.13	35	HETATM	4135	0	HOH	103	21.079	17.166 18.929	1.00	32.40
W		HETATM	4136	0	HOH	104	25.810	-5.921 22.506	1.00	37.69
		HETATM	4137	0	HOH	105	22.493	-1.311 34.465	1.00	49.94
10		HETATM	4138	0	HOH	106	19.317	10.977 38.703	1.00	40.60
10		HETATM	4139	0	HOH	107	4.479	13.951 3.045	1.00	45.33
134	40	HETATM	4140	0	HOH	108	20.418	19.353 34.044	1.00	42.18
		HETATM	4141	0	HOH	109	-3.065	8.936 14.062	1.00	38.41
		HETATM	4142	0	HOH	110	26.856	-4.674-10.940	1.00	55.67
		HETATM	4143	0	HOH	111	2.032	-6.387 5.614	1.00	42.23
		HETATM	4144	0	HOH	112	0.601	0.228-17.268	1.00	40.57
	45	HETATM	4145	0	HOH	113	4.903	13.488-14.050	1.00	47.72
		HETATM	4146	0	HOH	114	3.986	16.140 -0.960	1.00	40.66
		HETATM	4147	ō	HOH	115	12.968	-19.561 2.741	1.00	40.76
		HETATM	4148	o	HOH	116	7.170	15.583 2.599	1.00	43.69
		HETATM	4149	ō	HOH	117	-1.966	10.606 3.572	1.00	52.63
	50	HETATM	4150	o	HOH	118	29.030	10.644 6.707	1.00	42.54
	50	HETATM	4151	0	HOH	119	0.468	4.354 8.374	1.00	38.69
		HETATM	4151	0	HOH		29.086			
						120		17.119 19.272	1.00	45.51
		HETATM	4153	0	HOH	121	24.614	17.609 20.174	1.00	53.55
		HETATM	4154	0	HOH	122	-15.318	0.362 26.686	1.00	36.77
	55	HETATM	4155	0	HOH	123	-3.857	-24.786 28.325	1.00	39.64
		HETATM	4156	0	HOH	124	21.728	22.178 31.983	1.00	43.73
		HETATM	4157	0	HOH	125	31.650	-7.370 21.642	1.00	40.53
		HETATM	4158	0	HOH	126	25.421	10.436 21.161	1.00	32.31
		HETATM	4159	0	HOH	127	10.317	-9.457 12.998	1.00	37.77
	60	HETATM	4160	0	HOH	128	22.723	14.887 15.427	1.00	47.90
		HETATM	4161	0	HOH	129	6.702	9.556 37.596	1.00	47.81
		HETATM	4162	0	HOH	130	27.987	13.557 7.167	1.00	41.15

5	HETATM	4163	0	HOH	131	30.798	16.499 7.588	1.00	58.47
	HETATM	4164	0	HOH	132	10.071	-0.571-20.393	1.00	38.79
	HETATM	4165	0	HOH	133	9.562	8.334-21.392	1.00	36.80
	HETATM	4166	0	HOH	134	6.712	6.058 8.822	1.00	37.43
	HETATM	4167	0	HOH	135	5.927	8.454 10.594	1.00	42.34
10	HETATM	4168	0	HOH	136	4.472	6.306 10.973	1.00	37.35
	HETATM	4169	0	HOH	137	6.792	7.721 7.051	1.00	47.23
	HETATM	4170	0	HOH	138	24.513	11.582 33.724	1.00	45.55
	HETATM	4171	0	HOH	139	-2.528	-20.361 12.354	1.00	52.13
	HETATM	4172	0	HOH	140	-7.864	7.706 19.248	1.00	47.82
15	HETATM	4173	0	HOH	141	11.577	-16.962 24.398	1.00	39.43
	HETATM	4174	0	HOH	142	18.087	12.263 -5.507	1.00	33.36
	HETATM	4175	0	HOH	143	-6.816	-14.190 10.674	1.00	51.32
	HETATM	4176	0	HOH	144	-7.377	-16.701 33.528	1.00	57.11
	HETATM	4177	0	HOH	145	-5.379	-20.107 32.689	1.00	43.01
20	HETATM	4178	0	HOH	146	8.766	-7.947-16.274	1.00	49.96
	HETATM	4179	0	HOH	147	10.946	-7.937-18.142	1.00	55.67
	END								

Appendix 3

Atomic Coordinates for Human ERa Complexed With OHT

		CRYST1	58.2	42 58.	242	277.46	7 90.00	90.00	120.00	P 65	2 2 12
	10										
		ORIGX1		00000		0000	0.00000				
		ORIGX2		00000		0000	0.00000				
		ORIGX3		00000		0000	1.00000				
		SCALE1		17170		9913	0.00000				
	15	SCALE2		00000		.9826	0.00000		000		
		SCALE3	0.0	00000	0.00	0000	0.00360	1 0.00	000		
		ATOM	1	CB	LEU	306	6.638	11.502	3.989	1.00	61.20
		ATOM	2	C	LEU	306	7.381	10.684	6.231	1.00	61.47
	20	ATOM	3	0	LEU	306	6.407	11.020	6.905	1.00	62.09
		ATOM	4	N	LEU	306	6.369	9.128	4.588	1.00	62.32
		ATOM	5	CA	LEU	306	7.232	10.330	4.754	1.00	61.30
		ATOM	6	N	ALA	307	8.609	10.605	6.730	1.00	60.52
		MOTA	7	CA	ALA	307	8.891	10.912	8.125	1.00	58.77
	25	ATOM	8	CB	ALA	307	10.318	10.501	8.465	1.00	59.70
43		ATOM	9	C	ALA	307	8.692	12.393	8.429	1.00	57.51
i'U		ATOM	10	0	ALA	307	8.451	12.770	9.574	1.00	57.64
10		ATOM	11	N	LEU	308	8.789	13.228	7.400	1.00	55.82
- Inh		ATOM	12	CA	LEU	308	8.638	14.668	7.573	1.00	56.62
14	30	ATOM	13	CB	LEU	308	9.298	15.402	6.406	1.00	57.48
100		ATOM	14	CG	LEU	308	10.637	14.822	5.948	1.00	59.17
34		ATOM	15	CD1	LEU	308	10.474	14.189	4.569	1.00	60.38
26		ATOM	16	CD2	LEU	308	11.694	15.920	5.933	1.00	58.46
175.4		ATOM	17	C	LEU	308	7.190	15.130	7.710	1.00	56.51
la!	35	ATOM	18	0	LEU	308	6.935	16.307	7.961	1.00	55.58
1,1		ATOM	19	N	SER	309	6.246	14.208	7.546	1.00	57.04
(15)		ATOM	20	CA	SER	309	4.828	14.544	7.657	1.00	56.46
1		ATOM	21	CB	SER	309	4.034	13.896	6.514	1.00	56.79
1.00	40	ATOM	22	OG	SER	309	4.071	12.479	6.588	1.00	57.23
	40	ATOM	23	C	SER	309	4.261	14.095	9.003	1.00	56.13
		ATOM	24	0	SER	309	3.166	14.507	9.398	1.00	55.17
		ATOM	25	N	LEU	310	5.016	13.257	9.706	1.00	54.31
		ATOM	26	CA	LEU	310	4.591	12.749	11.004	1.00	53.55
	4.5	ATOM	27	CB	LEU	310	5.651	11.811	11.582	1.00	54.40
	45	ATOM	28	CG	LEU	310	5.586	10.333	11.189	1.00	56.49
		ATOM	29	CD1	LEU	310	5.530	10.200	9.676	1.00	57.06
		ATOM	30	CD2	LEU	310	6.809	9.610	11.739	1.00	57.28
		ATOM	31	C	LEU	310	4.330	13.865	12.003	1.00	53.18
		ATOM	32	0	LEU	310	4.993	14.905	11.984	1.00	53.17
	50	MOTA	33	N	THR	311	3.352	13.641	12.874	1.00	51.71
		ATOM	34	CA	THR	311	3.017	14.604	13.912	1.00	49.93
		MOTA	35	CB	THR	311	1.527	14.554	14.275	1.00	48.96
		ATOM	36	OG1	THR	311	1.242	13.311	14.930	1.00	47.20
		ATOM	37	CG2	THR	311	0.666	14.688	13.027	1.00	50.99
	55	ATOM	38	C	THR	311	3.815	14.201	15.145	1.00	48.84
		MOTA	39	0	THR	311	4.371	13.103	15.197	1.00	46.66
		ATOM	40	N	ALA	312	3.857	15.078	16.141	1.00	48.76
		ATOM	41	CA	ALA	312	4.590	14.798	17.369	1.00	47.75
	60	ATOM	42	CB	ALA	312	4.359	15.910	18.378	1.00	47.06
	ου	ATOM	43	C	ALA	312	4.171	13.460	17.964	1.00	47.41
		ATOM	44	0	ALA	312	5.009	12.609	18.262	1.00	45.52

	5	ATOM	45	N	ASP	313	2.868	13.275	18.143	1.00	47.58
		ATOM	46	CA	ASP	313	2.367	12.032	18.714	1.00	47.63
		ATOM	47	CB	ASP	313	0.848	12.100	18.879	1.00	
		ATOM	48	CG	ASP	313	0.430	12.872	20.118	1.00	56.21
		ATOM	49	OD1	ASP	313	1.314	13.234	20.929	1.00	56.38
	10	ATOM	50	OD2	ASP	313	-0.785	13.117	20.282	1.00	59.15
		ATOM	51	C	ASP	313	2.745	10.846	17.835	1.00	43.93
		ATOM	52	Ö	ASP	313	2.959	9.741	18.330	1.00	44.77
		ATOM	53	N	GLN	314	2.826	11.081	16.531	1.00	44.52
		ATOM	54	CA	GLN	314	3.182	10.028	15.588	1.00	44.73
	15	ATOM	55	CB	GLN	314	2.849		14.156		
	13	ATOM	56	CG	GLN	314	1.534	10.464		1.00	45.05
								9.886	13.626	1.00	48.47
		MOTA	57	CD	GLN	314	0.982	10.646	12.428	1.00	50.37
		ATOM	58	OE1	GLN	314	1.649	11.515	11.856	1.00	49.38
	20	ATOM	59	NE2	GLN	314	-0.248	10.318	12.043	1.00	51.74
	20	ATOM	60	C	GLN	314	4.673	9.722	15.707	1.00	43.26
		ATOM	61	0	GLN	314	5.100	8.580	15.555	1.00	43.93
		ATOM	62	N	MET	315	5.459	10.757	15.980	1.00	42.29
		ATOM	63	CA	MET	315	6.901	10.606	16.130	1.00	41.26
	0.5	ATOM	64	CB	MET	315	7.565	11.985	16.224	1.00	42.43
7005	25	ATOM	65	CG	MET	315	9.082	11.939	16.356	1.00	42.34
Ü		ATOM	66	SD	MET	315	9.906	11.190	14.925	1.00	46.22
11		ATOM	67	CE	MET	315	9.547	12.408	13.680	1.00	37.32
n		ATOM	68	C	MET	315	7.218	9.791	17.379	1.00	38.89
Euch		ATOM	69	0	MET	315	8.002	8.841	17.335	1.00	40.02
1d	30	ATOM	70	N	VAL	316	6.599	10.165	18.491	1.00	37.65
Į.i.		ATOM	71	CA	VAL	316	6.819	9.476	19.756	1.00	39.56
144		ATOM	72	CB	VAL	316	6.023	10.136	20.897	1.00	39.22
1)		ATOM	73	CG1	VAL	316	6.245	9.373	22.192	1.00	44.43
1000	25	MOTA	74	CG2	VAL	316	6.446	11.583	21.059	1.00	41.04
1,1,1	35	ATOM	75	C	VAL	316	6.404	8.012	19.664	1.00	40.04
1,1		ATOM	76	0	VAL	316	7.141	7.117	20.077	1.00	37.86
(154) 1554		ATOM	77	N	SER	317	5.215	7.767	19.127	1.00	41.90
Ď		MOTA	78	CA	SER	317	4.733	6.400	18.997	1.00	41.68
0		MOTA	79	CB	SER	317	3.311	6.402	18.415	1.00	43.85
100	40	ATOM	80	OG	SER	317	3.225	5.631	17.230	1.00	49.38
		ATOM	81	C	SER	317	5.696	5.601	18.114	1.00	39.72
		ATOM	82	0	SER	317	6.011	4.446	18.407	1.00	40.21
		MOTA	83	N	ALA	318	6.182	6.220	17.043	1.00	38.35
	4.5	ATOM	84	CA	ALA	318	7.114	5.540	16.153	1.00	36.96
	45	ATOM	85	CB	ALA	318	7.485	6.448	14.986	1.00	37.92
		ATOM	86	C	ALA	318	8.375	5.137	16.920	1.00	38.31
		ATOM	87	0	ALA	318	8.820	3.992	16.844	1.00	33.94
		MOTA	88	N	LEU	319	8.938	6.089	17.664	1.00	36.92
		ATOM	89	CA	LEU	319	10.161	5.854	18.438	1.00	38.56
	50	ATOM	90	CB	LEU	319	10.660	7.174	19.040	1.00	40.86
		MOTA	91	CG	LEU	319	11.136	8.264	18.071	1.00	41.25
		ATOM	92	CD1	LEU	319	11.714	9.440	18.857	1.00	44.30
		MOTA	93	CD2	LEU	319	12.182	7.693	17.140	1.00	42.61
		ATOM	94	C	LEU	319	9.965	4.826	19.549	1.00	38.33
	55	ATOM	95	0	LEU	319	10.779	3.916	19.729	1.00	33.91
		ATOM	96	N	LEU	320	8.879	4.982	20.297	1.00	37.39
		ATOM	97	CA	LEU	320	8.567	4.067	21.387	1.00	41.55
		ATOM	98	CB	LEU	320	7.239	4.467	22.049	1.00	38.47
		ATOM	99	CG	LEU	320	7.236	5.582	23.099	1.00	44.81
	60	ATOM	100	CD1	LEU	320	5.876	5.634	23.802	1.00	44.96
		ATOM	101	CD2	LEU	320	8.334	5.332	24.112	1.00	43.36
		MOTA	102	C	LEU	320	8.466	2.642	20.843	1.00	41.11

	5	ATOM	103	0	LEU	320	8.971	1.697	21.443	1.00	41.87
		ATOM	104	N	ASP	321	7.812	2.504	19.696	1.00	43.94
		ATOM	105	CA	ASP	321	7.613	1.210	19.053	1.00	44.77
		ATOM	106	CB	ASP	321	6.669	1.372	17.860	1.00	48.39
		ATOM	107	CG	ASP	321	5.206	1.318	18.255	1.00	52.39
	10	ATOM	108	OD1	ASP	321	4.901	1.422	19.464	1.00	53.56
		ATOM	109	OD2	ASP	321	4.357	1.172	17.346	1.00	55.81
		ATOM	110	C	ASP	321	8.911	0.565	18.568	1.00	44.37
		ATOM	111	0	ASP	321	9.030	-0.661	18.533	1.00	44.67
		ATOM	112	N	ALA	322	9.878	1.395	18.193	1.00	40.75
	15	ATOM	113	CA	ALA	322	11.153	0.905	17.686	1.00	37.81
		ATOM	114	CB	ALA	322	11.772	1.954	16.776	1.00	38.07
		ATOM	115	C	ALA	322	12.148	0.513	18.769	1.00	35.52
		ATOM	116	0	ALA	322	13.219	-0.020	18.473	1.00	36.11
		ATOM	117	N	GLU	323	11.799	0.768	20.022	1.00	35.61
	20	ATOM	118	CA	GLU	323	12.704	0.460	21.117	1.00	36.39
		ATOM	119	CB	GLU	323	12.042	0.768	22.459	1.00	35.09
		ATOM	120	CG	GLU	323	12.209	2.210	22.899	1.00	37.93
		ATOM	121	CD	GLU	323	13.657	2.569	23.200	1.00	37.29
		ATOM	122	OE1	GLU	323	14.313	3.173	22.326	1.00	34.21
	25	ATOM	123	OE2	GLU	323	14.134	2.245	24.309	1.00	38.02
	1000	ATOM	124	C	GLU	323	13.205	-0.978	21.110	1.00	38.01
	0	ATOM	125	0	GLU	323	12.425	-1.931	20.999	1.00	38.37
	11	ATOM	126	N	PRO	324	14.527	-1.151	21.225	1.00	36.03
	esi.	ATOM	127	CD	PRO	324	15.522	-0.069	21.225	1.00	36.69
	30	ATOM	128	CA	PRO	324	15.158	-2.474	21.240		36.42
	30	ATOM	129	CB	PRO	324	16.633	-2.474	21.240	1.00	35.75
	sels	ATOM		CG	PRO	324					
	4	ATOM	130	C	PRO	324	16.811	-0.807	21.610 22.583	1.00	35.46
	Si		131	0		324	14.940	-3.162		1.00	35.75 34.97
-	35	ATOM	132	N	PRO	325	14.616	-2.517	23.580	1.00	
	M 33	ATOM	133		PRO		15.134	-4.485	22.631	1.00	35.24
		ATOM	134	CD	PRO	325	15.530	-5.386	21.534	1.00	37.02
	3	ATOM ATOM	135 136	CA CB	PRO PRO	325 325	14.942 14.753	-5.208 -6.652	23.889	1.00	34.65 35.83
	Ď	ATOM	137	CG	PRO	325		-6.743		1.00	
	□ 40		138	C	PRO		15.589		22.200	1.00	34.88
	- 40	ATOM		0	PRO	325	16.132	-5.070	24.824		
		ATOM	139		ILE	325 326	17.237	-4.723	24.399	1.00	29.92
		MOTA MOTA	140 141	N CA	ILE	326	15.899 16.975	-5.322 -5.265	26.106 27.075	1.00	33.62 35.02
		ATOM	141	CB	ILE	326	16.458	-4.891	28.473	1.00	38.11
	45	ATOM			ILE	326					
	43		143	CG2 CG1	ILE	326	17.557	-5.110	29.504	1.00	38.70
		ATOM	144				15.987	-3.431	28.466		40.48
		ATOM	145	CD1	ILE	326	16.035	-2.747	29.815	1.00	42.96
		MOTA	146	C	ILE	326	17.567	-6.668	27.103	1.00	34.14
	50	MOTA	147	0	ILE	326	16.875	-7.634	27.427	1.00	34.88
	50	MOTA	148	N	LEU	327	18.840	-6.784	26.745	1.00	29.64
		ATOM	149	CA	LEU	327	19.493	-8.083	26.716	1.00	29.54
		MOTA	150	CB	LEU	327	20.528	-8.135	25.587	1.00	27.76
		MOTA	151	CG	LEU	327	19.978	-7.800	24.196	1.00	29.02
		MOTA	152	CD1	LEU	327	21.068	-7.993	23.139	1.00	28.76
	55	MOTA	153	CD2	LEU	327	18.775	-8.688	23.891	1.00	31.26
		MOTA	154	C	LEU	327	20.156	-8.438	28.030	1.00	31.21
		MOTA	155	0	LEU	327	20.393	-7.578	28.891	1.00	30.12
		MOTA	156	N	TYR	328	20.445	-9.725	28.181	1.00	30.99
		MOTA	157	CA	TYR	328	21.087	-10.229	29.381	1.00	30.95
	60	MOTA	158	CB	TYR	328	20.409	-11.520	29.842	1.00	33.38
		ATOM	159	CG	TYR	328	19.194	-11.272	30.686	1.00	33.05
		MOTA	160	CD1	TYR	328	19.253	-11.398	32.071	1.00	31.92

	5	ATOM	161	CE1	TYR	328	18.152 -11.114	32.864	1.00	36.01
		ATOM	162	CD2	TYR	328	17.996 -10.862	30.110	1.00	36.05
		ATOM	163	CE2	TYR	328	16.880 -10.574	30.899	1.00	37.27
		ATOM	164	CZ	TYR	328	16.973 -10.702	32.274	1.00	37.66
		ATOM	165	OH	TYR	328	15.896 -10.39		1.00	44.66
	10	ATOM	166	C	TYR	328	22.529 -10.520		1.00	33.66
		ATOM	167	o	TYR	328	22.884 -10.744		1.00	34.78
		ATOM	168	N	SER	329	23.359 -10.496			
									1.00	33.97
		ATOM	169	CA	SER	329	24.767 -10.800		1.00	37.29
	1.5	ATOM	170	CB	SER	329	25.526 -10.342		1.00	36.51
	15	ATOM	171	OG	SER	329	26.787 -10.969		1.00	37.13
		ATOM	172	C	SER	329	24.835 -12.31		1.00	40.43
		ATOM	173	0	SER	329	23.980 -13.028		1.00	40.11
		ATOM	174	N	GLU	330	25.845 -12.813	29.128	1.00	41.40
		MOTA	175	CA	GLU	330	25.992 -14.242	28.928	1.00	47.43
	20	ATOM	176	CB	GLU	330	26.423 -14.524	27.484	1.00	48.64
		ATOM	177	CG	GLU	330	25.278 -14.870	26.542	1.00	50.20
		ATOM	178	CD	GLU	330	25.765 -15.405	25.198	1.00	53.25
		ATOM	179	OE1	GLU	330	25.909 -16.640	25.062	1.00	53.27
		ATOM	180	OE2	GLU	330	26.004 -14.590		1.00	51.80
	25	ATOM	181	C	GLU	330	26.999 -14.852		1.00	49.67
		ATOM	182	ō	GLU	330	28.207 -14.741		1.00	50.11
123		ATOM	183	N	TYR	331	26.498 -15.493		1.00	53.62
11		ATOM	184	CA	TYR	331	27.373 -16.130		1.00	58.16
40				CB						
- de	30	ATOM	185		TYR	331	28.092 -15.078		1.00	59.55
1,1	30	ATOM	186	CG	TYR	331	27.239 -14.460		1.00	63.08
and s		ATOM	187	CD1	TYR	331	26.656 -13.205		1.00	64.50
1		ATOM	188	CE1	TYR	331	25.864 -12.630		1.00	65.99
81		MOTA	189	CD2	TYR	331	27.010 -15.128		1.00	63.52
(ton	2.5	ATOM	190	CE2	TYR	331	26.219 -14.563		1.00	65.60
L	35	MOTA	191	CZ	TYR	331	25.648 -13.314		1.00	67.20
		ATOM	192	OH	TYR	331	24.855 -12.753		1.00	67.40
T T		ATOM	193	C	TYR	331	26.603 -17.080		1.00	59.05
£		ATOM	194	0	TYR	331	25.393 -16.942	33.002	1.00	59.22
		ATOM	195	N	ASP	332	27.320 -18.045	33.387	1.00	61.62
D	40	ATOM	196	CA	ASP	332	26.719 -19.026	34.281	1.00	64.20
		ATOM	197	CB	ASP	332	27.681 -20.194	34.500	1.00	65.99
		ATOM	198	CG	ASP	332	26.961 -21.516	34.648	1.00	68.11
		ATOM	199	OD1	ASP	332	27.575 -22.564	34.351	1.00	69.54
		ATOM	200	OD2	ASP	332	25.781 -21.505	35.060	1.00	67.40
	45	ATOM	201	C	ASP	332	26.393 -18.371		1.00	63.33
		ATOM	202	0	ASP	332	27.292 -18.073		1.00	63.90
		ATOM	203	N	PRO	333	25.096 -18.148		1.00	63.64
		ATOM	204	CD	PRO	333	23.945 -18.509		1.00	64.35
		ATOM	205	CA	PRO	333	24.677 -17.521		1.00	63.52
	50	ATOM	206	CB	PRO	333	23.165 -17.333		1.00	63.53
	50									
		ATOM	207	CG	PRO	333	22.866 -17.611		1.00	64.15
		ATOM	208	C	PRO	333	25.010 -18.419		1.00	63.29
		MOTA	209	0	PRO	333	25.129 -17.964		1.00	63.28
		MOTA	210	N	THR	334	25.160 -19.704		1.00	64.26
	55	ATOM	211	CA	THR	334	25.475 -20.697		1.00	66.09
		ATOM	212	CB	THR	334	24.929 -22.080		1.00	66.90
		ATOM	213	OG1	THR	334	25.571 -22.513	37.439	1.00	68.06
		ATOM	214	CG2	THR	334	23.423 -22.012	38.411	1.00	67.57
		ATOM	215	C	THR	334	26.982 -20.804	39.269	1.00	65.67
	60	ATOM	216	0	THR	334	27.432 -21.323	40.289	1.00	64.77
		ATOM	217	N	ARG	335	27.759 -20.308	38.313	1.00	65.65
		ATOM	218	CA	ARG	335	29.214 -20.360	38.421	1.00	66.60
							226			
							220			

	5	ATOM	219	CB	ARG	335	29.835 -20	.500	37.030	1.00	66.74
		ATOM	220	C	ARG	335	29.757 -19	.113	39.123	1.00	67.09
		ATOM	221	0	ARG	335	29.100 -18	.071	39.148	1.00	67.31
		MOTA	222	N	PRO	336	30.968 -19	.207	39.702	1.00	67.62
		ATOM	223	CD	PRO	336	31.820 -20	.408	39.713	1.00	67.30
	10	ATOM	224	CA	PRO	336	31.601 -18	.086	40.410	1.00	67.42
		ATOM	225	CB	PRO	336	32.982 -18	.621	40.783	1.00	66.43
		ATOM	226	CG	PRO	336		.097	40.779	1.00	67.52
		ATOM	227	C	PRO	336		. 828	39.561	1.00	68.26
		ATOM	228	ō	PRO	336		.895	38.371	1.00	69.04
	15	ATOM	229	N	PHE	337		.681	40.183	1.00	69.49
		ATOM	230	CA	PHE	337		.408	39.480	1.00	71.39
		ATOM	231	CB	PHE	337		.323	40.294	1.00	72.31
		ATOM	232	CG	PHE	337		.924	39.921	1.00	73.21
		ATOM	233	CD1	PHE	337	30.632 -11		38.833	1.00	72.82
	20	ATOM	234	CD2	PHE	337	32.191 -11		40.653	1.00	73.43
	20	ATOM	235	CE1	PHE	337		.993	38.479	1.00	73.43
		ATOM	236	CE2	PHE	337		. 950	40.306	1.00	73.20
		ATOM	237	CEZ	PHE	337		.323		1.00	72.90
									39.217		
	25	ATOM	238	C	PHE	337	32.985 -14		39.245	1.00	71.38
(1)	23	ATOM	239	0	PHE	337		.487	38.189	1.00	71.56
164		ATOM	240	N	SER	338		. 273	40.241	1.00	71.53
173		ATOM	241	CA	SER	338		. 947	40.172	1.00	70.98
(5)		ATOM	242	CB	SER	338	35.957 -14		41.414	1.00	70.43
jus.	20	ATOM	243	OG	SER	338		.818	41.679	1.00	69.59
N	30	ATOM	244	C	SER	338		504	38.924	1.00	71.20
jat.		MOTA	245	0	SER	338		.972	38.475	1.00	71.35
4		ATOM	246	N	GLU	339	35.368 -15		38.369	1.00	70.20
93 37		MOTA	247	CA	GLU	339	35.930 -16		37.183	1.00	69.48
(2)		ATOM	248	CB	GLU	339		. 585	36.971	1.00	71.07
1,12	35	MOTA	249	CG	GLU	339		.740	37.656	1.00	72.60
1,1,1		MOTA	250	CD	GLU	339	35.382 -20		37.318	1.00	74.26
D.		MOTA	251	OE1	GLU	339	34.786 -20		36.227	1.00	73.51
		MOTA	252	OE2	GLU	339	35.496 -21		38.144	1.00	76.44
1		MOTA	253	C	GLU	339	35.770 -15		35.910	1.00	68.15
Feed	40	MOTA	254	0	GLU	339	36.722 -15		35.144	1.00	68.99
		ATOM	255	N	ALA	340	34.562 -14		35.694	1.00	64.41
		MOTA	256	CA	ALA	340	34.246 -14		34.507	1.00	60.69
		ATOM	257	CB	ALA	340		.709	34.523	1.00	61.17
		ATOM	258	C	ALA	340	35.096 -12		34.326	1.00	57.00
	45	MOTA	259	0	ALA	340	35.634 -12		35.287	1.00	57.46
		ATOM	260	N	SER	341	35.215 -12	.388	33.076	1.00	52.15
		ATOM	261	CA	SER	341	35.972 -11		32.736	1.00	46.53
		ATOM	262	CB	SER	341	36.839 -11	.439	31.497	1.00	48.64
		MOTA	263	OG	SER	341	37.184 -10	.226	30.846	1.00	46.48
	50	ATOM	264	C	SER	341	34.957 -10	.087	32.444	1.00	43.52
		ATOM	265	0	SER	341	34.090 -10	.248	31.589	1.00	39.92
		MOTA	266	N	MET	342	35.052 -8	.978	33.166	1.00	41.24
		ATOM	267	CA	MET	342	34.121 -7	. 875	32.960	1.00	42.46
		ATOM	268	CB	MET	342	34.449 -6	.723	33.912	1.00	45.61
	55	ATOM	269	CG	MET	342	33.228 -6.	.089	34.560	1.00	52.39
		MOTA	270	SD	MET	342	31.791 -7.	201	34.631	1.00	57.92
		ATOM	271	CE	MET	342	31.999 -7.	.881	36.239	1.00	56.18
		ATOM	272	C	MET	342	34.124 -7.	365	31.516	1.00	40.22
		ATOM	273	0	MET	342		.121	30.938	1.00	39.23
	60	ATOM	274	N	MET	343		204	30.930	1.00	38.72
		ATOM	275	CA	MET	343		708	29.558	1.00	38.50
		ATOM	276	CB	MET	343		318	29.216	1.00	41.15
							227				
							221				

	5	ATOM	277	CG	MET	343	37.022	-5.749	27.804	1.00	40.31
	,		278	SD	MET	343	36.032	-4.260	27.427	1.00	45.23
		ATOM ATOM	279	CE	MET	343	36.032	-3.358	28.987	1.00	40.45
		ATOM	280	C	MET	343	34.880	-7.741	28.561	1.00	35.36
		ATOM	281	0	MET	343	34.368	-7.384	27.501	1.00	35.51
	10		282	и	GLY	344	35.017	-9.020	28.902	1.00	35.51
	10	ATOM	283	CA	GLY	344	34.533	-10.072	28.024	1.00	33.41
		ATOM		CA	GLY	344	33.015	-10.072	28.024	1.00	31.74
		ATOM ATOM	284 285	0	GLY	344	32.359	-10.063	27.019	1.00	29.58
		ATOM	286	N	LEU	345	32.459	-9.860	29.238	1.00	32.89
	15	ATOM	287	CA	LEU	345	31.011	-9.804	29.415	1.00	34.95
	15	ATOM	288	CB	LEU	345	30.665	-9.631	30.902	1.00	37.56
		ATOM	289	CG	LEU	345	30.942	-10.774	31.883	1.00	43.03
		ATOM	290	CD1	LEU	345	30.537	-10.357	33.297	1.00	41.57
		ATOM	291	CD2	LEU	345	30.164	-11.998	31.449	1.00	42.80
	20	ATOM	292	C	LEU	345	30.430	-8.614	28.633	1.00	33.71
		ATOM	293	0	LEU	345	29.479	-8.757	27.868	1.00	30.29
		ATOM	294	N	LEU	346	31.021	-7.443	28.843	1.00	30.20
		ATOM	295	CA	LEU	346	30.569	-6.217	28.193	1.00	32.00
		ATOM	296	CB	LEU	346	31.317	-5.016	28.771	1.00	28.16
	25	ATOM	297	CG	LEU	346	31.091	-4.767	30.269	1.00	29.84
13		ATOM	298	CD1	LEU	346	31.815	-3.498	30.668	1.00	29.98
10		ATOM	299	CD2	LEU	346	29.614	-4.644	30.581	1.00	33.97
17,1		ATOM	300	C	LEU	346	30.732	-6.250	26.682	1.00	30.70
Ø		ATOM	301	ō	LEU	346	29.869	-5.765	25.955	1.00	29.13
100	30	ATOM	302	N	THR	347	31.839	-6.816	26.212	1.00	30.47
N		ATOM	303	CA	THR	347	32.086	-6.911	24.781	1.00	30.93
inda A. J		ATOM	304	CB	THR	347	33.472	-7.501	24.497	1.00	29.97
14		ATOM	305	OG1	THR	347	34.481	-6.604	24.982	1.00	35.40
20		ATOM	306	CG2	THR	347	33.666	-7.707	23.004	1.00	33.58
	35	ATOM	307	C	THR	347	31.036	-7.804	24.122	1.00	31.97
1,1,3		ATOM	308	0	THR	347	30.516	-7.486	23.049	1.00	30.75
1.0		MOTA	309	N	ASN	348	30.737	-8.926	24.768	1.00	29.31
100		MOTA	310	CA	ASN	348	29.757	-9.868	24.242	1.00	32.63
D.		MOTA	311	CB	ASN	348	29.767	-11.161	25.065	1.00	31.64
12.3	40	MOTA	312	CG	ASN	348	28.646	-12.117	24.662	1.00	39.14
		MOTA	313	OD1	ASN	348	27.549	-12.078	25.220	1.00	41.91
		ATOM	314	ND2	ASN	348	28.920	-12.970	23.683	1.00	42.05
		ATOM	315	С	ASN	348	28.361	-9.251	24.262	1.00	29.02
		ATOM	316	0	ASN	348	27.558	-9.477	23.353	1.00	32.76
	45	ATOM	317	N	LEU	349	28.078	-8.467	25.298	1.00	28.74
		ATOM	318	CA	LEU	349	26.782	-7.811	25.421	1.00	28.58 26.56
		ATOM	319	CB	LEU	349	26.650	-7.148 -6.328	26.795 27.050	1.00	33.67
		ATOM	320	CG	LEU	349	25.376 24.140	-6.328	26.840	1.00	28.82
	50	ATOM	321	CD1	LEU	349		-7.199	28.471	1.00	33.11
	50	ATOM ATOM	322 323	CD2 C	LEU	349 349	25.392 26.638	-6.762	24.319	1.00	28.07
			323	0		349	25.616	-6.703	23.629	1.00	25.22
		ATOM ATOM	325	N	LEU ALA	350	27.675	-5.941	24.157	1.00	28.50
		ATOM	326	CA	ALA	350	27.668	-4.886	23.148	1.00	28.46
	55	ATOM	327	CB	ALA	350	28.972	-4.094	23.209	1.00	28.12
	55	ATOM	328	C	ALA	350	27.468	-5.461	21.750	1.00	28.75
		ATOM	329	0	ALA	350	26.649	-4.958	20.983	1.00	30.90
		ATOM	330	N	ASP	351	28.213	-6.509	21.420	1.00	27.20
		ATOM	331	CA	ASP	351	28.093	-7.143	20.112	1.00	29.75
	60	ATOM	332	CB	ASP	351	29.036	-8.345	20.010	1.00	34.16
	~ ~	ATOM	333	CG	ASP	351	30.498	-7.940	19.978	1.00	37.50
		ATOM	334	OD1	ASP	351	31.354	-8.831	20.148	1.00	37.55
							22		- · · · -	-	-
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	5	ATOM	335	OD2	ASP	351	30.789	-6.738	19.784	1.00	35.50
		MOTA	336	C	ASP	351	26.661	-7.600	19.813	1.00	30.52
		MOTA	337	0	ASP	351	26.193	-7.458	18.687	1.00	27.77
		ATOM	338	N	ARG	352	25.968	-8.150	20.811	1.00	27.18
		ATOM	339	CA	ARG	352	24.593	-8.602	20.605	1.00	26.21
	10	ATOM	340	CB	ARG	352	24.148	-9.534	21.752	1.00	26.52
		ATOM	341	CG	ARG	352	24.567	-10.991	21.532	1.00	31.03
		ATOM	342	CD	ARG	352	24.128	-11.911	22.666	1.00	29.80
				NE	ARG	352	24.898	-11.675	23.879	1.00	30.44
		ATOM	343	CZ	ARG	352	24.364	-11.363	25.054	1.00	31.68
	15	ATOM	344								
	13	ATOM	345	NH1	ARG	352	23.050	-11.251	25.177	1.00	31.18
		MOTA	346	NH2	ARG	352	25.144	-11.148	26.104	1.00	32.03
		MOTA	347	C	ARG	352	23.642	-7.411	20.502	1.00	27.16
		ATOM	348	0	ARG	352	22.702	-7.426	19.708	1.00	26.65
		MOTA	349	N	GLU	353	23.896	-6.370	21.291	1.00	24.30
	20	MOTA	350	CA	GLU	353	23.045	-5.178	21.261	1.00	26.39
		ATOM	351	CB	GLU	353	23.461	-4.204	22.365	1.00	24.91
		MOTA	352	CG	GLU	353	23.147	-4.669	23.771	1.00	27.93
		ATOM	353	CD	GLU	353	23.425	-3.587	24.795	1.00	30.71
		ATOM	354	OE1	GLU	353	24.564	-3.534	25.304	1.00	30.09
780	25	ATOM	355	OE2	GLU	353	22.506	-2.789	25.085	1.00	30.53
(")		ATOM	356	C	GLU	353	23.131	-4.456	19.920	1.00	24.27
vi)		ATOM	357	0	GLU	353	22.169	-3.826	19.467	1.00	28.71
i'U		ATOM	358	N	LEU	354	24.296	-4.540	19.293	1.00	26.61
1,0		ATOM	359	CA	LEU	354	24.522	-3.872	18.017	1.00	26.62
100	30	ATOM	360	CB	LEU	354	25.952	-4.121	17.543	1.00	26.36
116	30							-3.257	16.351	1.00	29.24
enin.		MOTA	361	CG	LEU	354	26.372	-3.257	16.722	1.00	26.59
14.		ATOM	362	CD1	LEU	354	26.243				
91		ATOM	363	CD2	LEU	354	27.794	-3.607	15.962	1.00	28.88
fine.	2.5	ATOM	364	C	LEU	354	23.559	-4.300	16.926	1.00	27.72
L	35	MOTA	365	0	LEU	354	23.074	-3.475	16.152	1.00	24.00
1.7		MOTA	366	N	VAL	355	23.291	-5.598	16.854	1.00	28.82
U		MOTA	367	CA	VAL	355	22.386	-6.125	15.844	1.00	29.45
10		ATOM	368	CB	VAL	355	22.259	-7.655	15.975	1.00	31.76
in the		MOTA	369	CG1	VAL	355	21.423	-8.205	14.834	1.00	33.55
1333	40	MOTA	370	CG2	VAL	355	23.649	-8.282	15.998	1.00	31.36
		MOTA	371	C	VAL	355	21.020	-5.499	16.035	1.00	27.71
		MOTA	372	0	VAL	355	20.382	-5.039	15.080	1.00	29.61
		ATOM	373	N	HIS	356	20.580	-5.473	17.288	1.00	27.76
		MOTA	374	CA	HIS	356	19.291	-4.906	17.627	1.00	28.35
	45	ATOM	375	CB	HIS	356	18.936	-5.231	19.079	1.00	31.12
		ATOM	376	CG	HIS	356	18.602	-6.675	19.307	1.00	35.93
		ATOM	377	CD2	HIS	356	19.352	-7.700	19.779	1.00	33.95
		MOTA	378	ND1	HIS	356	17.363	-7.208	19.018	1.00	36.62
		ATOM	379	CE1	HIS	356	17.364	-8.499	19.304	1.00	33.33
	50	ATOM	380	NE2	HIS	356	18.559	-8.823	19.767	1.00	32.16
	50	ATOM	381	C	HIS	356	19.300	-3.398	17.412	1.00	28.25
		ATOM	382	0	HIS	356	18.272	-2.812	17.100	1.00	28.99
										1.00	
		MOTA	383	N	MET	357	20.457	-2.765	17.574		25.31
		MOTA	384	CA	MET	357	20.526	-1.322	17.369	1.00	24.63
	55	MOTA	385	CB	MET	357	21.902	-0.789	17.766	1.00	23.61
		MOTA	386	CG	MET	357	22.011	0.736	17.699	1.00	24.66
		MOTA	387	SD	MET	357	23.732	1.290	17.859	1.00	27.30
		MOTA	388	CE	MET	357	24.140	0.672	19.514	1.00	23.62
		MOTA	389	C	MET	357	20.256	-1.011	15.898	1.00	24.83
	60	MOTA	390	0	MET	357	19.619	-0.003	15.569	1.00	26.78
		MOTA	391	N	ILE	358	20.757	-1.874	15.020	1.00	26.25
		ATOM	392	CA	ILE	358	20.553	-1.721	13.576	1.00	30.33

	5	ATOM	393	CB	ILE	358	21.204	-2.888	12.789	1.00	33.86
		ATOM	394	CG2	ILE	358	20.759	-2.860	11.334	1.00	33.68
		ATOM	395	CG1	ILE	358	22.728	-2.799	12.874	1.00	36.89
		ATOM	396	CD1	ILE	358	23.299	-1.469	12.451	1.00	39.10
		ATOM	397	C	ILE	358	19.055	-1.721	13.310	1.00	32.20
	10										
	10	ATOM	398	0	ILE	358	18.519	-0.817	12.662	1.00	32.02
		ATOM	399	N	ASN	359	18.379	-2.748	13.814	1.00	33.12
		ATOM	400	CA	ASN	359	16.945	-2.861	13.638	1.00	33.35
		ATOM	401	CB	ASN	359	16.434	-4.101	14.363	1.00	37.59
		ATOM	402	CG	ASN	359	16.739	-5.374	13.627	1.00	44.38
	15	ATOM	403	OD1	ASN	359	17.045	-5.329	12.437	1.00	47.35
		ATOM	404	ND2	ASN	359	16.673	-6.508	14.320	1.00	42.48
		ATOM	405	C	ASN	359	16.224	-1.634	14.149	1.00	32.74
					ASN	359					
		ATOM	406	0			15.261	-1.163	13.530	1.00	31.39
	20	MOTA	407	N	TRP	360	16.706	-1.104	15.264	1.00	27.92
	20	ATOM	408	CA	TRP	360	16.102	0.087	15.842	1.00	29.47
		ATOM	409	CB	TRP	360	16.703	0.347	17.228	1.00	27.66
		ATOM	410	CG	TRP	360	16.522	1.747	17.707	1.00	30.40
		ATOM	411	CD2	TRP	360	17.493	2.801	17.657	1.00	27.54
		ATOM	412	CE2	TRP	360	16.888	3.954	18.204	1.00	29.42
V.	25	ATOM	413	CE3	TRP	360	18.819	2.883	17.205	1.00	28.37
100	**	ATOM	414	CD1	TRP	360	15.399	2.284	18.264	1.00	27.75
13	Ü	ATOM	415	NE1	TRP	360	15.609	3.611	18.566	1.00	30.84
2	W										
0	O .	ATOM	416	CZ2	TRP	360	17.558	5.180	18.310	1.00	27.74
1	# 20	ATOM	417	CZ3	TRP	360	19.488	4.106	17.309	1.00	24.49
44		ATOM	418	CH2	TRP	360	18.853	5.232	17.858	1.00	25.09
ş.,		ATOM	419	C	TRP	360	16.312	1.296	14.926	1.00	27.90
5,		ATOM	420	0	TRP	360	15.360	2.002	14.581	1.00	28.83
		ATOM	421	N	ALA	361	17.559	1.520	14.523	1.00	28.25
51		ATOM	422	CA	ALA	361	17.894	2.637	13.645	1.00	29.20
£	35	MOTA	423	CB	ALA	361	19.346	2.539	13.220	1.00	28.89
1		ATOM	424	C	ALA	361	17.006	2.685	12.403	1.00	31.08
1	الله ا	ATOM	425	ō	ALA	361	16.531	3.746	12.011	1.00	31.30
1	1	ATOM	426	N	LYS	362	16.795	1.526	11.783	1.00	30.93
1	Ö	ATOM	427	CA	LYS	362	15.981	1.443	10.581	1.00	34.15
48			428	CB							
	- 40	ATOM			LYS	362	16.012	0.016	10.023	1.00	33.67
		ATOM	429	CG	LYS	362	17.252	-0.281	9.198	1.00	39.40
		ATOM	430	CD	LYS	362	17.547	-1.774	9.136	1.00	43.60
		ATOM	431	CE	LYS	362	18.852	-2.046	8.389	1.00	47.06
		ATOM	432	NZ	LYS	362	19.178	-3.507	8.288	1.00	50.34
	45	ATOM	433	C	LYS	362	14.545	1.872	10.815	1.00	35.81
		ATOM	434	0	LYS	362	13.821	2.168	9.859	1.00	37.95
		ATOM	435	N	ARG	363	14.134	1.921	12.079	1.00	34.23
		ATOM	436	CA	ARG	363	12.770	2.313	12.409	1.00	36.04
		ATOM	437	CB	ARG	363	12.178	1.307	13.391	1.00	36.71
	50	ATOM	438	CG	ARG	363	12.169	-0.110	12.827	1.00	40.36
	50	ATOM	439	CD	ARG	363	11.468	-1.086	13.746	1.00	42.17
		ATOM	440	NE	ARG	363	10.161	-0.586	14.158	1.00	45.19
		ATOM	441	CZ	ARG	363	9.314	-1.262	14.929	1.00	49.41
		MOTA	442	NH1	ARG	363	9.642	-2.467	15.374	1.00	48.02
	55	ATOM	443	NH2	ARG	363	8.143	-0.729	15.261	1.00	51.54
		ATOM	444	C	ARG	363	12.654	3.743	12.943	1.00	37.40
		ATOM	445	0	ARG	363	11.567	4.199	13.303	1.00	38.22
		ATOM	446	N	VAL	364	13.785	4.442	13.002	1.00	35.66
		ATOM	447	CA	VAL	364	13.804	5.836	13.431	1.00	34.06
	60	ATOM	448	CB	VAL	364	15.231	6.271	13.827	1.00	33.87
		ATOM	449	CG1	VAL	364	15.293	7.779	13.995	1.00	31.08
				CG2	VAL	364					
		ATOM	450	CG2	VAL	364	15.641	5.571	15.113	1.00	31.30

	5	ATOM	451	C	VAL	364	13.360	6.591	12.171	1.00	33.19
		ATOM	452	0	VAL	364	14.028	6.531	11.146	1.00	33.04
		MOTA	453	N	PRO	365	12.225	7.310	12.234	1.00	34.69
		ATOM	454	CD	PRO	365	11.359	7.492	13.413	1.00	34.19
		ATOM	455	CA	PRO	365	11.724	8.050	11.069	1.00	35.96
	10	ATOM	456	CB	PRO	365	10.608	8.918	11.645	1.00	36.59
		ATOM	457	CG	PRO	365	10.135	8.157	12.842	1.00	39.59
		ATOM	458	C	PRO	365	12.756	8.878	10.321	1.00	37.19
		ATOM	459	0	PRO	365	13.430	9.726	10.907	1.00	40.29
			460	N		366		8.624	9.023		
	15	ATOM			GLY		12.878			1.00	34.78
	13	MOTA	461	CA	GLY	366	13.816	9.371	8.212	1.00	33.54
		MOTA	462	C	GLY	366	15.168	8.722	8.007	1.00	34.26
		ATOM	463	0	GLY	366	15.858	9.035	7.034	1.00	37.15
		MOTA	464	N	PHE	367	15.554	7.814	8.901	1.00	33.13
		ATOM	465	CA	PHE	367	16.860	7.164	8.787	1.00	32.04
	20	ATOM	466	CB	PHE	367	17.138	6.291	10.016	1.00	30.22
		ATOM	467	CG	PHE	367	18.544	5.773	10.080	1.00	30.60
		ATOM	468	CD1	PHE	367	18.827	4.446	9.751	1.00	31.94
		ATOM	469	CD2	PHE	367	19.589	6.601	10.485	1.00	29.20
		ATOM	470	CE1	PHE	367	20.133	3.950	9.828	1.00	28.30
les.	25	ATOM	471	CE2	PHE	367	20.896	6.122	10.568	1.00	28.12
(3		ATOM	472	CZ	PHE	367	21.171	4.791	10.240	1.00	25.41
10		ATOM	473	C	PHE	367	17.033	6.333	7.524	1.00	31.46
145		ATOM	474	ō	PHE	367	18.073	6.405	6.883	1.00	32.30
111		ATOM	475	N	VAL	368	16.027	5.541	7.165	1.00	35.20
-de	30	ATOM	476	CA	VAL	368	16.123	4.718	5.959	1.00	38.98
11/4	50	ATOM	477	CB	VAL	368	15.076	3.584	5.945	1.00	40.61
j.A		ATOM	478	CG1	VAL	368		2.447	6.843	1.00	
145.3							15.543				41.48
21		ATOM	479	CG2	VAL	368	13.717	4.113	6.390	1.00	41.60
13	25	ATOM	480	C	VAL	368	15.965	5.523	4.673	1.00	40.06
141	35	ATOM	481	0	VAL	368	16.156	4.992	3.579	1.00	41.66
U		ATOM	482	N	ASP	369	15.608	6.798	4.798	1.00	38.65
(100		ATOM	483	CA	ASP	369	15.465	7.646	3.621	1.00	37.15
10		MOTA	484	CB	ASP	369	14.700	8.929	3.954	1.00	39.89
ind ind		ATOM	485	CG	ASP	369	13.254	8.671	4.302	1.00	45.59
134	40	MOTA	486	OD1	ASP	369	12.686	7.672	3.806	1.00	46.34
		MOTA	487	OD2	ASP	369	12.681	9.472	5.074	1.00	49.13
		ATOM	488	C	ASP	369	16.855	8.010	3.136	1.00	34.91
		MOTA	489	0	ASP	369	17.038	8.431	1.995	1.00	34.25
		MOTA	490	N	LEU	370	17.838	7.841	4.016	1.00	31.76
	45	ATOM	491	CA	LEU	370	19.229	8.153	3.705	1.00	28.08
		ATOM	492	CB	LEU	370	20.020	8.339	5.003	1.00	28.81
		ATOM	493	CG	LEU	370	19.523	9.395	6.000	1.00	28.74
		ATOM	494	CD1	LEU	370	20.315	9.275	7.299	1.00	30.81
		ATOM	495	CD2	LEU	370	19.693	10.792	5,404	1.00	29.77
	50	ATOM	496	C	LEU	370	19.884	7.043	2.893	1.00	31.25
		ATOM	497	Ö	LEU	370	19.341	5.943	2.784	1.00	31.78
		ATOM	498	N	THR	371	21.052	7.333	2.331	1.00	28.86
			499	CA			21.793	6.336			32.90
		ATOM			THR	371			1.569	1.00	
		ATOM	500	CB	THR	371	22.979	6.944	0.818	1.00	33.44
	55	ATOM	501	OG1	THR	371	23.880	7.523	1.766	1.00	34.59
		ATOM	502	CG2	THR	371	22.514	8.002	-0.178	1.00	32.63
		ATOM	503	C	THR	371	22.373	5.315	2.539	1.00	35.31
		MOTA	504	0	THR	371	22.536	5.591	3.733	1.00	31.27
		MOTA	505	N	LEU	372	22.702	4.141	2.015	1.00	34.34
	60	MOTA	506	CA	LEU	372	23.273	3.073	2.822	1.00	35.46
		ATOM	507	CB	LEU	372	23.518	1.841	1.944	1.00	37.73
		ATOM	508	CG	LEU	372	24.362	0.704	2.515	1.00	42.43
							231				
							35.				

	5	ATOM	509	CD1	LEU	372	23.690	0.145	3.757	1.00	45.60
		ATOM	510	CD2	LEU	372	24.534	-0.383	1.455	1.00	44.29
		ATOM	511	C	LEU	372	24.587	3.548	3.444	1.00	36.95
		ATOM	512	0	LEU	372	24.813	3.374	4.643	1.00	35.57
		ATOM	513	N	HIS	373	25.442	4.159	2.627	1.00	35.68
	10	ATOM	514	CA	HIS	373	26.729	4.656	3.099	1.00	36.60
	10										
		ATOM	515	CB	HIS	373	27.506	5.282	1.935	1.00	44.01
		ATOM	516	CG	HIS	373	28.538	6.280	2.360	1.00	50.69
		ATOM	517	CD2	HIS	373	29.857	6.138	2.636	1.00	54.69
		MOTA	518	ND1	HIS	373	28.246	7.613	2.561	1.00	53.77
	15	ATOM	519	CE1	HIS	373	29.339	8.248	2.945	1.00	57.09
		ATOM	520	NE2	HIS	373	30.331	7.376	2.999	1.00	57.23
		ATOM	521	C	HIS	373	26.575	5.669	4.244	1.00	36.22
		ATOM	522	0	HIS	373	27.350	5.650	5.201	1.00	33.05
		ATOM	523	N	ASP	374	25.580	6.549	4.148	1.00	32.03
	20	ATOM	524	CA	ASP	374	25.342	7.541	5.196	1.00	30.76
	20			CB	ASP		24.354	8.603	4.713		
		MOTA	525			374				1.00	30.12
		MOTA	526	CG	ASP	374	25.018	9.672	3.860	1.00	35.83
		MOTA	527	OD1	ASP	374	26.264	9.744	3.842	1.00	34.39
		MOTA	528	OD2	ASP	374	24.291	10.440	3.199	1.00	35.39
1112	25	MOTA	529	C	ASP	374	24.805	6.876	6.472	1.00	30.33
12		MOTA	530	0	ASP	374	25.152	7.275	7.587	1.00	27.04
113		MOTA	531	N	GLN	375	23.944	5.877	6.309	1.00	25.71
144		ATOM	532	CA	GLN	375	23.403	5.157	7.454	1.00	26.68
co		ATOM	533	CB	GLN	375	22.424	4.077	6.993	1.00	29.70
1.4	30	ATOM	534	CG	GLN	375	21.101	4.616	6.484	1.00	29.16
4		ATOM	535	CD	GLN	375	20.219	3.514	5.940	1.00	35.87
100		ATOM	536	OE1	GLN	375	20.155	2.426	6.510	1.00	30.97
1		ATOM	537	NE2	GLN	375	19.541	3.785	4.827	1.00	34.51
81			538		GLN	375	24.556	4.502	8.214	1.00	25.51
(3	35	MOTA		C							
1,0	33	MOTA	539	0	GLN	375	24.585	4.513	9.442	1.00	28.14
1.U		MOTA	540	N	VAL	376	25.504	3.938	7.475	1.00	26.62
156		MOTA	541	CA	VAL	376	26.659	3.281	8.071	1.00	29.24
975		ATOM	542	CB	VAL	376	27.531	2.597	7.003	1.00	29.66
- der		MOTA	543	CG1	VAL	376	28.812	2.071	7.635	1.00	28.29
12.0	40	MOTA	544	CG2	VAL	376	26.745	1.469	6.341	1.00	29.90
		ATOM	545	C	VAL	376	27.526	4.285	8.821	1.00	30.87
		ATOM	546	0	VAL	376	27.953	4.029	9.948	1.00	30.09
		ATOM	547	N	HIS	377	27.785	5.428	8.191	1.00	28.05
		ATOM	548	CA	HIS	377	28.602	6.457	8.814	1.00	28.68
	45	ATOM	549	CB	HIS	377	28.792	7.639	7.864	1.00	30.26
		ATOM	550	CG	HIS	377	29.508	8.791	8.488	1.00	33.89
		ATOM	551	CD2	HIS	377	29.073	10.017	8.863	1.00	34.99
		ATOM	552	ND1	HIS	377	30.846	8.740	8.823	1.00	37.01
		ATOM	553	CE1	HIS	377	31.201	9.884	9.377	1.00	34.79
	50										
	50	MOTA	554	NE2	HIS	377	30.144	10.677	9.413	1.00	34.95
		ATOM	555	C	HIS	377	27.983	6.954	10.114	1.00	25.13
		MOTA	556	0	HIS	377	28.677	7.102	11.115	1.00	25.93
		ATOM	557	N	LEU	378	26.678	7.206	10.107	1.00	24.58
		MOTA	558	CA	LEU	378	26.015	7.695	11.315	1.00	26.40
	55	MOTA	559	CB	LEU	378	24.542	8.001	11.027	1.00	26.29
		ATOM	560	CG	LEU	378	24.291	9.180	10.073	1.00	28.06
		ATOM	561	CD1	LEU	378	22.778	9.353	9.869	1.00	27.66
		ATOM	562	CD2	LEU	378	24.911	10.458	10.642	1.00	30.08
		ATOM	563	C	LEU	378	26.120	6.695	12.459	1.00	28.55
	60	ATOM	564	0	LEU	378	26.379	7.075	13.605	1.00	24.76
	00	ATOM	565	N	LEU	379	25.919	5.414	12.153	1.00	24.29
		ATOM	566	CA	LEU	379	26.000	4.388	13.182	1.00	27.03

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	5	ATOM	567	CB	LEU	379	25.401	3.073	12.667	1.00	28.53
		ATOM ATOM	568 569	CG CD1	LEU	379 379	23.875	3.023	12.845	1.00	30.29
		ATOM	570	CD1	LEU	379	23.248 23.563	1.943 2.759	11.963 14.312	1.00	33.04 29.45
		ATOM	571	CDZ	LEU	379	27.430	4.176	13.670	1.00	27.18
	10	ATOM	572	0	LEU	379	27.653	3.979	14.866	1.00	25.95
		ATOM	573	N	GLU	380	28.402	4.236	12.762	1.00	25.86
		ATOM	574	CA	GLU	380	29.786	4.054	13.173	1.00	27.58
		MOTA	575	CB	GLU	380	30.730	4.036	11.968	1.00	30.36
		ATOM	576	CG	GLU	380	32.172	3.785	12.380	1.00	37.98
	15	ATOM	577	CD	GLU	380	33.080	3.471	11.210	1.00	45.23
		ATOM	578	OE1	GLU	380	32.869	4.048	10.120	1.00	42.99
		MOTA	579	OE2	GLU	380	34.004	2.646	11.386	1.00	45.79
		MOTA	580	C	GLU	380	30.218	5.159	14.133	1.00	27.50
		MOTA	581	0	GLU	380	31.056	4.937	15.010	1.00	26.67
	20	MOTA	582	N	ACYS	381	29.637	6.339	13.965	0.75	24.89
		ATOM	583	N	BCYS	381	29.645	6.352	13.980	0.25	25.79
		MOTA	584	CA	ACYS	381	29.969	7.466	14.826	0.75	24.12
		MOTA	585	CA	BCYS	381	29.993	7.481	14.847	0.25	24.86
	25	ATOM	586	CB	ACYS	381	29.621	8.781	14.122	0.75	25.96
TAN	23	ATOM ATOM	587 588	CB SG	BCYS ACYS	381 381	29.766 30.698	8.814 9.192	14.115 12.732	0.25	25.62 31.63
+0		ATOM	589	SG	BCYS	381	30.898	10.312	15.059	0.75	25.40
11		ATOM	590	C	ACYS	381	29.237	7.422	16.162	0.75	22.07
1.0		ATOM	591	C	BCYS	381	29.211	7.498	16.159	0.25	23.97
2120	30	ATOM	592	0	ACYS	381	29.812	7.730	17.206	0.75	21.97
1		ATOM	593	o	BCYS	381	29.724	7.940	17.187	0.25	23.99
le di		ATOM	594	N	ALA	382	27.974	7.012	16.128	1.00	23.41
14		ATOM	595	CA	ALA	382	27.140	7.015	17.318	1.00	22.83
8) (13)		ATOM	596	CB	ALA	382	25.785	7.587	16.948	1.00	25.50
la.	35	ATOM	597	C	ALA	382	26.913	5.755	18.131	1.00	25.39
(,,)		MOTA	598	0	ALA	382	26.374	5.837	19.234	1.00	23.09
Total Cont		ATOM	599	N	TRP	383	27.311	4.602	17.615	1.00	25.98
1150		ATOM	600	CA	TRP	383	27.026	3.354	18.318	1.00	23.80
Д		ATOM	601	CB	TRP	383	27.669	2.172	17.580	1.00	22.52
1012	40	ATOM	602	CG	TRP	383	29.130	2.054	17.762	1.00	24.42
		ATOM ATOM	603 604	CD2 CE2	TRP	383 383	29.797 31.182	1.347	18.803 18.579	1.00	27.31 28.24
		ATOM	605	CE3	TRP	383	29.360	0.609	19.912	1.00	27.37
		ATOM	606	CD1	TRP	383	30.102	2.578	16.965	1.00	24.58
	45	ATOM	607	NE1	TRP	383	31.342	2.239	17.446	1.00	27.35
		ATOM	608	CZ2	TRP	383	32.133	0.909	19.420	1.00	28.76
		ATOM	609	CZ3	TRP	383	30.305	0.039	20.745	1.00	28.09
		ATOM	610	CH2	TRP	383	31.674	0.191	20.496	1.00	29.77
		MOTA	611	C	TRP	383	27.356	3.309	19.802	1.00	23.54
	50	MOTA	612	0	TRP	383	26.526	2.866	20.584	1.00	22.90
		MOTA	613	N	LEU	384	28.542	3.765	20.211	1.00	20.37
		MOTA	614	CA	LEU	384	28.864	3.713	21.640	1.00	22.41
		MOTA	615	CB	LEU	384	30.369	3.890	21.883	1.00	24.98
		MOTA	616	CG	LEU	384	30.824	3.645	23.336	1.00	27.33
	55	ATOM	617	CD1	LEU	384	30.273	2.305	23.853	1.00	29.71
		MOTA	618	CD2	LEU	384	32.336	3.648	23.398	1.00	26.07
		ATOM	619	C	LEU	384	28.075	4.732	22.453	1.00	19.44
		ATOM ATOM	620 621	O N	LEU GLU	384 385	27.706 27.807	4.458 5.909	23.595 21.885	1.00	23.24
	60	ATOM	622	CA	GLU	385	27.807	6.895	22.612	1.00	21.32
	00	ATOM	623	CB	GLU	385	26.861	8.177	21.797	1.00	21.32
		ATOM	624	CG	GLU	385	28.115	9.020	21.705	1.00	21.61

	5	MOTA	625	CD	GLU	385	27.882	10.256	20.860	1.00	29.53
		ATOM	626	OE1	GLU	385	27.374	11.256	21.401	1.00	30.54
		MOTA	627	OE2	GLU	385	28.188	10.219	19.658	1.00	29.97
		ATOM	628	C	GLU	385	25.616	6.292	22.836	1.00	22.26
		ATOM	629	ō	GLU	385	25.022	6.438	23.902	1.00	22.26
	10	ATOM	630	N	ILE	386	25.101	5.617	21.812	1.00	22.03
		ATOM	631	CA	ILE	386	23.779	4.995	21.896	1.00	22.74
		ATOM	632	CB	ILE	386	23.328	4.455	20.498	1.00	22.88
		ATOM	633	CG2	ILE	386	22.009	3.647	20.438	1.00	23.85
		ATOM	634	CG1	ILE	386	23.085	5.651	19.561	1.00	25.05
	15										
	13	MOTA	635	CD1	ILE	386	22.994	5.297	18.078	1.00	26.42
		ATOM	636	C	ILE	386	23.766	3.897	22.961	1.00	22.50
		MOTA	637	0	ILE	386	22.823	3.818	23.746	1.00	24.75
		MOTA	638	N	LEU	387	24.810	3.071	23.020	1.00	22.25
	20	MOTA	639	CA	LEU	387	24.868	2.030	24.051	1.00	22.95
	20	ATOM	640	CB	LEU	387	26.096	1.132	23.864	1.00	24.61
		MOTA	641	CG	LEU	387	26.070	0.194	22.654	1.00	23.21
		MOTA	642	CD1	LEU	387	27.297	-0.709	22.705	1.00	25.36
		MOTA	643	CD2	LEU	387	24.791	-0.631	22.652	1.00	26.29
		MOTA	644	C	LEU	387	24.944	2.660	25.438	1.00	26.22
100	25	MOTA	645	0	LEU	387	24.287	2.204	26.386	1.00	23.55
in id	5	MOTA	646	N	MET	388	25.751	3.713	25.554	1.00	23.92
14	i i	MOTA	647	CA	MET	388	25.924	4.385	26.835	1.00	24.26
41	it S	ATOM	648	CB	MET	388	27.088	5.378	26.761	1.00	23.87
la la		MOTA	649	CG	MET	388	28.440	4.722	26.743	1.00	24.08
24	30	MOTA	650	SD	MET	388	29.726	5.992	26.736	1.00	27.70
Į		ATOM	651	CE	MET	388	31.139	5.041	27.078	1.00	21.74
34		ATOM	652	C	MET	388	24.660	5.094	27.321	1.00	23.33
		ATOM	653	0	MET	388	24.341	5.026	28.505	1.00	25.58
37	4	ATOM	654	N	ILE	389	23.935	5.775	26.436	1.00	24.62
1.0	35	ATOM	655	CA	ILE	389	22.729	6.440	26.905	1.00	24.03
4,8		ATOM	656	CB	ILE	389	22.132	7.439	25.852	1.00	27.01
Į,	j	ATOM	657	CG2	ILE	389	21.413	6.705	24.706	1.00	23.98
fine.		ATOM	658	CG1	ILE	389	21.185	8.402	26.584	1.00	25.49
1		ATOM	659	CD1	ILE	389	20.431	9.383	25.683	1.00	25.45
12	40	ATOM	660	C	ILE	389	21.694	5.401	27.349	1.00	26.54
		ATOM	661	0	ILE	389	20.938	5.631	28.294	1.00	22.58
		ATOM	662	N	GLY	390	21.679	4.247	26.687	1.00	27.14
		ATOM	663	CA	GLY	390	20.753	3.201	27.090	1.00	28.42
		ATOM	664	C	GLY	390	21.133	2.719	28.482	1.00	29.67
	45	ATOM	665	0	GLY	390	20.275	2.521	29.348	1.00	29.21
		ATOM	666	N	LEU	391	22.433	2.547	28.699	1.00	26.06
		ATOM	667	CA	LEU	391	22.955	2.091	29.983	1.00	29.23
		ATOM	668	CB	LEU	391	24.476	1.937	29.899	1.00	28.37
		ATOM	669	CG	LEU	391	25.206	1.656	31.210	1.00	30.81
	50	ATOM	670	CD1	LEU	391	24.717	0.332	31.793	1.00	25.73
		ATOM	671	CD2	LEU	391	26.709	1.619	30.958	1.00	25.25
		ATOM	672	C	LEU	391	22.603	3.070	31.104	1.00	30.84
		ATOM	673	ō	LEU	391	22.156	2.669	32.186	1.00	29.19
		ATOM	674	N	VAL	392	22.817	4.355	30.850	1.00	28.91
	55	ATOM	675	CA	VAL	392	22.506	5.369	31.851	1.00	28.86
	55	ATOM	676	CB	VAL	392	22.923	6.770	31.353	1.00	30.08
		ATOM	677	CG1	VAL	392	22.329	7.854	32.237	1.00	32.32
		ATOM	678	CG2	VAL	392	24.442	6.870	31.372	1.00	28.52
		ATOM	679	C	VAL	392	21.013	5.327	32.165	1.00	28.42
	60	ATOM	680	0	VAL	392	20.621	5.345	33.327	1.00	30.38
	00	ATOM	681	N	TRP	392	20.621	5.345	33.327	1.00	28.23
		ATOM	682	CA	TRP	393	18.732	5.186	31.125	1.00	29.70
		MI ON	002	CM	TKP	323	10./32	3.100	J⊥.∠6U	1.00	23.10

	5	3 50014	600	an.	mp p	202	10 000	F 046	29.906	1.00	30.09
	3	ATOM	683	CB	TRP	393	18.066	5.046			
		ATOM	684	CG	TRP	393	16.605	4.670	29.953	1.00	33.50
		ATOM	685	CD2	TRP	393	15.516	5.499	30.369	1.00	31.76
		ATOM	686	CE2	TRP	393	14.336	4.725	30.264	1.00	38.11
		ATOM	687	CE3	TRP	393	15.419	6.821	30.824	1.00	32.56
	10	ATOM	688	CD1	TRP	393	16.057	3.459	29.618	1.00	34.31
		MOTA	689	NE1	TRP	393	14.696	3.486	29.801	1.00	34.36
		ATOM	690	CZ2	TRP	393	13.073	5.233	30.597	1.00	37.93
		ATOM	691	CZ3	TRP	393	14.162	7.326	31.155	1.00	35.24
				CH2	TRP	393	13.007	6.531	31.039	1.00	37.77
	1.5	ATOM	692								
	15	ATOM	693	C	TRP	393	18.256	4.051	32.191	1.00	32.07
		ATOM	694	0	TRP	393	17.460	4.275	33.109	1.00	32.12
		ATOM	695	N	ARG	394	18.738	2.837	31.957	1.00	31.90
		ATOM	696	CA	ARG	394	18.288	1.729	32.787	1.00	36.63
		ATOM	697	CB	ARG	394	18.492	0.389	32.065	1.00	36.41
	20	ATOM	698	CG	ARG	394	19.914	0.009	31.764	1.00	36.50
		ATOM	699	CD	ARG	394	19.929	-1.132	30.748	1.00	36.34
		ATOM	700	NE	ARG	394	21.282	-1.561	30.417	1.00	33.97
		ATOM	701	CZ	ARG	394	21.864	-1.350	29.239	1.00	31.61
		ATOM	702	NH1	ARG	394	21.208	-0.715	28.281	1.00	32.42
	25	ATOM	703	NH2	ARG	394	23.098	-1.784	29.022	1.00	29.81
15.4	23										36.69
40		ATOM	704	C	ARG	394	18.911	1.697	34.180	1.00	
111		ATOM	705	0	ARG	394	18.445	0.966	35.048	1.00	37.07
120		ATOM	706	N	SER	395	19.954	2.492	34.395	1.00	33.63
Jick		ATOM	707	CA	SER	395	20.603	2.564	35.701	1.00	35.69
4	30	ATOM	708	CB	SER	395	22.112	2.784	35.540	1.00	32.94
inde		ATOM	709	OG	SER	395	22.696	1.811	34.688	1.00	32.37
1		ATOM	710	C	SER	395	20.010	3.713	36.531	1.00	36.44
		ATOM	711	0	SER	395	20.389	3.916	37.687	1.00	38.68
E(ATOM	712	N	MET	396	19.076	4.449	35.937	1.00	36.46
	35	ATOM	713	CA	MET	396	18.431	5.588	36.589	1.00	43.08
int	0.0	ATOM	714	CB	MET	396	17.275	6.104	35.725	1.00	43.87
1,1,1		ATOM	715	CG	MET	396	17.481	7.507	35.176	1.00	46.18
1.3				SD	MET	396	15.962	8.278	34.581	1.00	49.58
0		ATOM	716						36.065		53.58
:0	40	ATOM	717	CE	MET	396	14.988	8.298		1.00	
***	40	ATOM	718	C	MET	396	17.906	5.303	37.992	1.00	46.18
		ATOM	719	0	MET	396	18.125	6.089	38.913	1.00	46.34
		ATOM	720	N	GLU	397	17.215	4.180	38.152	1.00	49.39
		ATOM	721	CA	GLU	397	16.645	3.821	39.444	1.00	52.12
		ATOM	722	CB	GLU	397	15.296	3.130	39.246	1.00	55.34
	45	ATOM	723	CG	GLU	397	14.166	4.073	38.873	1.00	58.86
		ATOM	724	CD	GLU	397	13.195	3.448	37.891	1.00	63.28
		ATOM	725	OE1	GLU	397	13.660	2.925	36.854	1.00	64.68
		ATOM	726	OE2	GLU	397	11.972	3.475	38.155	1.00	65.39
		ATOM	727	C	GLU	397	17.548	2.933	40.283	1.00	52.75
	50	ATOM	728	0	GLU	397	17.071	2.187	41.139	1.00	53.96
	50								40.040	1.00	50.25
		ATOM	729	N	HIS	398	18.851	3.014			
		ATOM	730	CA	HIS	398	19.813	2.220	40.792	1.00	49.34
		ATOM	731	CB	HIS	398	20.271	1.018	39.963	1.00	52.04
		ATOM	732	CG	HIS	398	19.187	0.017	39.721	1.00	53.95
	55	ATOM	733	CD2	HIS	398	18.750	-1.022	40.472	1.00	53.92
		ATOM	734	ND1	HIS	398	18.374	0.054	38.608	1.00	55.91
		ATOM	735	CE1	HIS	398	17.482	-0.917	38.685	1.00	55.53
		ATOM	736	NE2	HIS	398	17.688	-1.585	39.806	1.00	55.81
		ATOM	737	C	HIS	398	20.999	3.084	41.196	1.00	47.44
	60	ATOM	738	ō	HIS	398	22.121	2.887	40.730	1.00	44.91
		ATOM	739	N	PRO	399	20.755	4.049	42.096	1.00	46.45
		ATOM	740	CD	PRO	399	19.443	4.300	42.721	1.00	47.27
		141 011	, = 0	CD	1100	3,5	13.113	1.500			

	5	MOTA	741	CA	PRO	399	21.785	4.968	42.586	1.00	45.35
		MOTA	742	CB	PRO	399	21.127	5.631	43.793	1.00	47.40
		MOTA	743	CG	PRO	399	19.660	5.561	43.504	1.00	47.72
		ATOM	744	C	PRO	399	23.086	4.270	42.958	1.00	44.70
		ATOM	745	0	PRO	399	23.078	3.233	43.627	1.00	46.46
	10	ATOM	746	N	GLY	400	24.202	4.840	42.509	1.00	41.57
	10	ATOM	747	CA	GLY	400	25.506	4.281	42.813	1.00	39.84
			748	C	GLY	400	25.907	3.047	42.022	1.00	37.85
		ATOM									
		ATOM	749	0	GLY	400	27.027	2.560	42.176	1.00	40.48
		ATOM	750	N	LYS	401	25.012	2.537	41.180	1.00	36.39
	15	MOTA	751	CA	LYS	401	25.315	1.344	40.390	1.00	34.47
		ATOM	752	CB	LYS	401	24.562	0.130	40.947	1.00	36.12
		ATOM	753	CG	LYS	401	24.633	-0.007	42.466	1.00	39.30
		ATOM	754	CD	LYS	401	24.288	-1.429	42.903	1.00	44.38
		ATOM	755	CE	LYS	401	24.459	-1.605	44.408	1.00	46.68
	20	ATOM	756	NZ	LYS	401	24.968	-2.969	44.747	1.00	53.37
		ATOM	757	C	LYS	401	24.969	1.485	38.911	1.00	32.34
		ATOM	758	0	LYS	401	24.141	2.308	38.531	1.00	31.16
		ATOM	759	N	LEU	402	25.612	0.663	38.086	1.00	28.52
		ATOM	760	CA	LEU	402	25.358	0.658	36.648	1.00	29.06
	25	ATOM	761	CB	LEU	402	26.661	0.847	35.867	1.00	29.26
Acres 1	23		762	CG	LEU	402	27.278	2.242	36.029	1.00	24.67
40		ATOM									
15		ATOM	763	CD1	LEU	402	28.623	2.310	35.310	1.00	27.47
100		ATOM	764	CD2	LEU	402	26.312	3.277	35.482	1.00	24.93
Ends	20	ATOM	765	C	LEU	402	24.755	-0.686	36.292	1.00	30.43
14	30	MOTA	766	0	LEU	402	25.367	-1.727	36.535	1.00	31.36
1		ATOM	767	N	LEU	403	23.552	-0.658	35.735	1.00	31.07
1		MOTA	768	CA	LEU	403	22.873	-1.880	35.335	1.00	32.96
		ATOM	769	CB	LEU	403	21.361	-1.693	35.434	1.00	33.86
fi) (m)		MOTA	770	CG	LEU	403	20.551	-2.991	35.415	1.00	39.29
la.	35	ATOM	771	CD1	LEU	403	20.584	-3.637	36.806	1.00	43.62
		ATOM	772	CD2	LEU	403	19.128	-2.689	34.998	1.00	41.32
W		ATOM	773	C	LEU	403	23.255	-2.218	33.899	1.00	30.06
100		ATOM	774	0	LEU	403	22.543	-1.870	32.956	1.00	31.63
133		ATOM	775	N	PHE	404	24.383	-2.893	33.733	1.00	29.19
9. D	40	ATOM	776	CA	PHE	404	24.834	-3.256	32.403	1.00	28.93
		ATOM	777	CB	PHE	404	26.201	-3.929	32.493	1.00	30.05
		ATOM	778	CG	PHE	404	27.305	-2.998	32.926	1.00	30.78
		ATOM	779	CD1	PHE	404	27.794	-3.033	34.228	1.00	32.91
		ATOM	780	CD2	PHE	404	27.734	-2.078	32.030	1.00	32.75
	45					404			34.638	1.00	34.73
	43	ATOM	781	CE1	PHE		28.816	-2.160			
		ATOM	782	CE2	PHE	404	28.864	-1.205	32.423	1.00	30.68
		ATOM	783	CZ	PHE	404	29.350	-1.242	33.727	1.00	31.43
		ATOM	784	C	PHE	404	23.809	-4.181	31.756	1.00	30.80
		ATOM	785	0	PHE	404	23.625	-4.175	30.538	1.00	28.09
	50	ATOM	786	N	ALA	405	23.138	-4.967	32.594	1.00	30.25
		ATOM	787	CA	ALA	405	22.104	-5.910	32.163	1.00	29.78
		MOTA	788	CB	ALA	405	22.745	-7.172	31.598	1.00	29.97
		ATOM	789	C	ALA	405	21.309	-6.237	33.429	1.00	31.95
		ATOM	790	0	ALA	405	21.785	-5.995	34.535	1.00	32.36
	55	ATOM	791	N	PRO	406	20.088	-6.779	33.288	1.00	34.40
		ATOM	792	CD	PRO	406	19.356	-7.102	32.053	1.00	35.81
		ATOM	793	CA	PRO	406	19.303	-7.101	34.490	1.00	36.41
		ATOM	794	CB	PRO	406	17.985	-7.654	33.935	1.00	35.38
		ATOM	795	CG	PRO	406	17.922	-7.153	32.519	1.00	36.49
	60			C		406	19.997	-8.084	35.433	1.00	37.32
	00	ATOM	796	0	PRO PRO	406	19.997	-8.084	36.626	1.00	38.34
		ATOM	797								
		MOTA	798	N	ASN	407	20.924	-8.877	34.902	1.00	36.69

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	5	ATOM	799	CA	ASN	407	21.652	-9.847	35.712	1.00	38.85
		ATOM	800	CB	ASN	407	21.582	-11.243	35.083	1.00	39.69
		ATOM	801	CG	ASN	407	22.232	-11.306	33.711	1.00	44.10
		ATOM	802	OD1	ASN	407	22.345	-10.296	33.009	1.00	37.78
		MOTA	803	ND2	ASN	407	22.660	-12.503	33.319	1.00	45.74
	10	ATOM	804	C	ASN	407	23.100	-9.435	35.874	1.00	38.12
		ATOM	805	0	ASN	407	23.965	-10.256	36.178	1.00	39.81
		ATOM	806	N	LEU	408	23.364	-8.149	35.671	1.00	37.80
		ATOM	807	CA	LEU	408	24.713	-7.631	35.799	1.00	36.89
		ATOM	808	CB	LEU	408	25.449	-7.720	34.459	1.00	36.09
	15	ATOM	809	CG	LEU	408	26.972	-7.609	34.550	1.00	35.08
		ATOM	810	CD1	LEU	408	27.525	-8.775	35.354	1.00	39.15
		ATOM	811	CD2	LEU	408	27.578	-7.587	33.158	1.00	36.85
		ATOM	812	C	LEU	408	24.670	-6.187	36.286	1.00	40.55
		ATOM	813	o	LEU	408	24.646	-5.248	35.491	1.00	38.29
	20	ATOM	814	N	LEU	409	24.644	-6.034	37.607	1.00	39.50
	20	ATOM	815	CA	LEU	409	24.606	-4.733	38.257	1.00	41.00
		ATOM	816	CB	LEU	409	23.392	-4.658	39.184	1.00	43.69
		ATOM		CG	LEU	409	23.392	-3.382	39.104	1.00	47.35
			817								
	25	ATOM	818	CD1	LEU	409	22.848	-2.233	39.058	1.00	47.09
(22)	23	MOTA	819	CD2	LEU	409	22.014	-3.603	40.976	1.00	49.38
143		ATOM	820	C	LEU	409	25.894	-4.566	39.060	1.00	41.80
		MOTA	821	0	LEU	409	26.178	-5.358	39.960	1.00	41.00
133		ATOM	822	N	LEU	410	26.676	-3.544	38.727	1.00	39.23
1-4		MOTA	823	CA	LEU	410	27.931	-3.296	39.423	1.00	40.45
44.1	30	MOTA	824	CB	LEU	410	29.106	-3.354	38.442	1.00	41.59
int.		MOTA	825	CG	LEU	410	29.457	-4.660	37.716	1.00	44.87
14		MOTA	826	CD1	LEU	410	30.972	-4.728	37.554	1.00	45.41
al .		MOTA	827	CD2	LEU	410	28.949	-5.872	38.484	1.00	47.02
100		MOTA	828	C	LEU	410	27.946	-1.944	40.132	1.00	40.67
1007	35	MOTA	829	0	LEU	410	27.361	-0.970	39.652	1.00	40.22
W		MOTA	830	N	ASP	411	28.610	-1.890	41.281	1.00	41.57
1.0		MOTA	831	CA	ASP	411	28.717	-0.640	42.025	1.00	42.69
(7)		MOTA	832	CB	ASP	411	28.490	-0.874	43.528	1.00	44.44
12		ATOM	833	CG	ASP	411	29.655	-1.578	44.210	1.00	46.70
D	40	ATOM	834	OD1	ASP	411	29.537	-1.849	45.426	1.00	51.44
		ATOM	835	OD2	ASP	411	30.680	-1.861	43.553	1.00	48.79
		ATOM	836	C	ASP	411	30.088	-0.016	41.779	1.00	43.70
		ATOM	837	0	ASP	411	30.933	-0.610	41.107	1.00	38.48
		ATOM	838	N	ARG	412	30.295	1.181	42.321	1.00	46.78
	45	ATOM	839	CA	ARG	412	31.554	1.905	42.171	1.00	49.97
		ATOM	840	CB	ARG	412	31.601	3.090	43.138	1.00	51.28
		ATOM	841	CG	ARG	412	30.971	4.364	42.614	1.00	54.77
		ATOM	842	CD	ARG	412	31.644	5.580	43.219	1.00	54.61
		ATOM	843	NE	ARG	412	33.071	5.615	42.912	1.00	56.53
	50	ATOM	844	CZ	ARG	412	33.827	6.708	42.985	1.00	61.90
	50	ATOM	845	NH1	ARG	412	33.291	7.866	43.356	1.00	63.48
		ATOM	846	NH2	ARG	412	35.120	6.645	42.682	1.00	61.21
		ATOM	847	C	ARG	412	32.771	1.026	42.429	1.00	50.29
								0.866			
		ATOM	848	0	ARG	412	33.628		41.561	1.00	51.02
	55	ATOM	849	N	ASN	413	32.844	0.469	43.633	1.00	51.94
		ATOM	850	CA	ASN	413	33.969	-0.375	44.021	1.00	53.15
		MOTA	851	CB	ASN	413	33.719	-0.980	45.403	1.00	55.88
		ATOM	852	CG	ASN	413	33.654	0.073	46.496	1.00	57.99
		ATOM	853	OD1	ASN	413	33.697	1.276	46.223	1.00	58.27
	60	ATOM	854	ND2	ASN	413	33.551	-0.375	47.742	1.00	57.90
		ATOM	855	C	ASN	413	34.235	-1.480	43.013	1.00	53.95
		ATOM	856	0	ASN	413	35.386	-1.743	42.659	1.00	53.67
							237	7			

	5	ATOM	857	N	GLN	414	33.173	-2.129	42.547	1.00	55.33
		ATOM	858	CA	GLN	414	33.326	-3.198	41.573	1.00	55.42
		ATOM	859	CB	GLN	414	31.991	-3.904	41.343	1.00	55.44
		ATOM	860	CG	GLN	414	31.645	-4.933	42.391	1.00	56.07
		ATOM	861	CD	GLN	414	30.203	-5.376	42.336	1.00	57.40
	10			OE1	GLN	414	29.296	-4.536	42.402	1.00	60.22
	10	MOTA	862								
		MOTA	863	NE2	GLN	414	29.973	-6.664	42.199	1.00	57.27
		ATOM	864	C	GLN	414	33.850	-2.630	40.259	1.00	55.51
		ATOM	865	0	GLN	414	34.654	-3.265	39.578	1.00	56.16
		MOTA	866	N	GLY	415	33.398	-1.430	39.910	1.00	57.07
	15	ATOM	867	CA	GLY	415	33.849	-0.806	38.680	1.00	58.51
		MOTA	868	C	GLY	415	35.350	-0.582	38.689	1.00	61.10
		ATOM	869	0	GLY	415	36.023	-0.748	37.671	1.00	59.47
		ATOM	870	N	LYS	416	35.877	-0.211	39.851	1.00	62.77
		ATOM	871	CA	LYS	416	37.305	0.041	40.011	1.00	65.49
	20	ATOM	872	CB	LYS	416	37.634	0.262	41.491	1.00	66.04
		ATOM	873	CG	LYS	416	38.121	1.663	41.823	1.00	68.71
		ATOM	874	CD	LYS	416	37.078	2.439	42.613	1.00	70.98
		ATOM	875	CE	LYS	416	37.404	2.448	44.100	1.00	71.84
										1.00	71.95
	25	MOTA	876	NZ	LYS	416	36.225	2.079	44.933		
3,43	25	MOTA	877	C	LYS	416	38.159	-1.105	39.472	1.00	66.41
		MOTA	878	0	LYS	416	39.361	-0.946	39.269	1.00	67.15
111		MOTA	879	N	CYS	417	37.538	-2.257	39.238	1.00	67.33
133		MOTA	880	CA	CYS	417	38.270	-3.414	38.741	1.00	68.16
to de		ATOM	881	CB	CYS	417	37.951	-4.642	39.602	1.00	70.88
34	30	MOTA	882	SG	CYS	417	38.592	-4.549	41.301	1.00	76.09
- Frank		ATOM	883	C	CYS	417	38.015	-3.736	37.270	1.00	67.54
1		ATOM	884	0	CYS	417	38.632	-4.653	36.720	1.00	68.48
		ATOM	885	N	VAL	418	37.111	-2.994	36.631	1.00	64.67
25		ATOM	886	CA	VAL	418	36.817	-3.226	35.218	1.00	59.97
£12.2	35	ATOM	887	CB	VAL	418	35.326	-2.917	34.879	1.00	59.60
1,1,5		ATOM	888	CG1	VAL	418	34.971	-1.503	35.284	1.00	59.13
141		ATOM	889	CG2	VAL	418	35.072	-3.121	33.391	1.00	54.85
Total		ATOM	890	C	VAL	418	37.739	-2.362	34.355	1.00	58.37
10		ATOM	891	0	VAL	418	37.799	-1.140	34.512	1.00	55.44
*D	40	ATOM	892	N	GLU	419	38.463	-3.012	33.450	1.00	56.02
	40		893	CA	GLU	419	39.403	-2.328	32.570	1.00	54.28
		ATOM		CB	GLU		40.149	-3.351	31.710	1.00	57.57
		ATOM	894			419					
		ATOM	895	CG	GLU	419	39.385	-3.779	30.468	1.00	60.87
	4.5	ATOM	896	CD	GLU	419	40.179	-4.722	29.584	1.00	63.34
	45	ATOM	897	OE1	GLU	419	40.432	-5.870	30.011	1.00	64.90
		MOTA	898	OE2	GLU	419	40.546	-4.313	28.462	1.00	63.18
		MOTA	899	C	GLU	419	38.761	-1.281	31.662	1.00	52.05
		MOTA	900	0	GLU	419	37.665	-1.481	31.131	1.00	49.82
		ATOM	901	N	GLY	420	39.465	-0.165	31.491	1.00	49.45
	50	ATOM	902	CA	GLY	420	38.983	0.908	30.642	1.00	46.22
		ATOM	903	C	GLY	420	37.895	1.767	31.254	1.00	44.55
		ATOM	904	0	GLY	420	37.417	2.705	30.619	1.00	42.08
		ATOM	905	N	MET	421	37.503	1.471	32.488	1.00	43.41
		ATOM	906	CA	MET	421	36.449	2.248	33.123	1.00	42.48
	55	ATOM	907	CB	MET	421	35.306	1.327	33.554	1.00	42.34
	55	ATOM	908	CG	MET	421	34.590	0.635	32.396	1.00	38.22
		ATOM	909	SD	MET	421	32.927	0.102	32.843	1.00	38.56
		ATOM	910	CE	MET	421	32.003	1.699	32.766	1.00	35.54
	CO	ATOM	911	C	MET	421	36.923	3.059	34.312	1.00	41.64
	60	ATOM	912	0	MET	421	36.113	3.512	35.111	1.00	39.77
		ATOM	913	N	VAL	422	38.232	3.256	34.430	1.00	43.42
		ATOM	914	CA	VAL	422	38.757	4.019	35.557	1.00	44.79

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	5	ATOM	915	CB	VAL	422	40.285	4.248	35.433	1.00	46.54
		ATOM	916	CG1	VAL	422	40.595	5.086	34.206	1.00	48.25
		MOTA	917	CG2	VAL	422	40.813	4.920	36.696	1.00	46.24
		ATOM	918	C	VAL	422	38.056	5.372	35.689	1.00	44.09
		MOTA	919	0	VAL	422	37.691	5.783	36.783	1.00	44.12
	10	ATOM	920	N	GLU	423	37.846	6.055	34.570	1.00	42.07
		MOTA	921	CA	GLU	423	37.192	7.356	34.616	1.00	40.24
		ATOM	922	CB	GLU	423	37.909	8.338	33.684	1.00	44.02
		ATOM	923	CG	GLU	423	39.411	8.467	33.893	1.00	50.04
		ATOM		CD	GLU	423		9.158	32.719	1.00	55.64
	15		924 925	OE1		423	40.096			1.00	
	13	MOTA			GLU		39.539	10.156	32.205		56.66
		MOTA	926	OE2	GLU	423	41.188	8.703	32.306	1.00	58.02
		ATOM	927	С	GLU	423	35.704	7.337	34.250	1.00	35.77
		ATOM	928	0	GLU	423	34.881	7.955	34.919	1.00	33.20
		MOTA	929	N	ILE	424	35.345	6.617	33.197	1.00	36.16
	20	MOTA	930	CA	ILE	424	33.949	6.643	32.771	1.00	31.63
		MOTA	931	CB	ILE	424	33.803	6.087	31.347	1.00	33.58
		ATOM	932	CG2	ILE	424	34.639	6.936	30.395	1.00	33.48
		MOTA	933	CG1	ILE	424	34.204	4.617	31.296	1.00	34.46
		MOTA	934	CD1	ILE	424	33.857	3.955	29.978	1.00	34.67
1000	25	MOTA	935	C	ILE	424	32.890	6.035	33.685	1.00	28.89
10		MOTA	936	0	ILE	424	31.729	6.443	33.632	1.00	26.49
IU		MOTA	937	N	PHE	425	33.261	5.091	34.542	1.00	29.26
(0		ATOM	938	CA	PHE	425	32.257	4.520	35.447	1.00	29.87
144		MOTA	939	CB	PHE	425	32.903	3.529	36.423	1.00	31.26
J	30	MOTA	940	CG	PHE	425	31.948	2.496	36.959	1.00	32.17
		ATOM	941	CD1	PHE	425	31.124	2.783	38.048	1.00	33.70
And N		ATOM	942	CD2	PHE	425	31.881	1.230	36.381	1.00	30.64
		MOTA	943	CE1	PHE	425	30.244	1.814	38.563	1.00	32.60
57		MOTA	944	CE2	PHE	425	31.010	0.256	36.881	1.00	31.55
	35	MOTA	945	CZ	PHE	425	30.189	0.549	37.973	1.00	33.34
W		MOTA	946	C	PHE	425	31.594	5.649	36.240	1.00	30.17
123		MOTA	947	0	PHE	425	30.368	5.774	36.276	1.00	26.71
(0)		ATOM	948	N	ASP	426	32.415	6.483	36.870	1.00	29.45
45		MOTA	949	CA	ASP	426	31.893	7.587	37.661	1.00	32.29
111	40	ATOM	950	CB	ASP	426	33.031	8.291	38.401	1.00	33.49
		ATOM	951	CG	ASP	426	33.455	7.546	39.655	1.00	39.42
		ATOM	952	OD1	ASP	426	32.767	6.574	40.038	1.00	38.35
		ATOM	953	OD2	ASP	426	34.480	7.934	40.256	1.00	39.58
		ATOM	954	C	ASP	426	31.133	8.592	36.806	1.00	29.02
	45	ATOM	955	0	ASP	426	30.154	9.175	37.257	1.00	31.34
		ATOM	956	N	MET	427	31.585	8.797	35.572	1.00	30.69
		ATOM	957	CA	MET	427	30.919	9.736	34.675	1.00	28.63
		ATOM	958	CB	MET	427	31.744	9.912	33.407	1.00	26.83
		ATOM	959	CG	MET	427	33.032	10.680	33.608	1.00	31.41
	50	ATOM	960	SD	MET	427	33.962	10.783	32.077	1.00	34.87
	50	ATOM	961	CE	MET	427	35.409	11.753	32.643	1.00	44.60
		ATOM	962	C	MET	427	29.526	9.202	34.324	1.00	28.70
		ATOM	963	0	MET	427	28.536	9.947	34.302	1.00	25.01
		ATOM	964	N	LEU	428	29.451	7.902	34.057	1.00	25.13
	55			CA	LEU	428		7.292	33.730	1.00	27.60
	33	ATOM	965				28.173 28.379				
		ATOM	966	CB	LEU	428		5.824	33.332	1.00	28.00
		ATOM	967	CG	LEU	428	29.039	5.682	31.957	1.00	26.99
		ATOM	968	CD1	LEU	428	29.678	4.303	31.782	1.00	27.80
	60	ATOM	969	CD2	LEU	428	27.995	5.927	30.894	1.00	25.33
	60	ATOM	970	C	LEU	428	27.210	7.412	34.916	1.00	29.59
		ATOM	971	0	LEU	428	26.041	7.743	34.743	1.00	27.07
		MOTA	972	N	LEU	429	27.701	7.147	36.126	1.00	30.40

	5	ATOM	973	CA	LEU	429	26.859	7.251	37.323	1.00	30.59
	3	ATOM	974	CB	LEU	429	27.675	6.884	38.571	1.00	31.76
		ATOM	975	CG	LEU	429	28.078	5.415	38.757	1.00	32.43
		ATOM	976	CD1	LEU	429	28.961	5.264	39.995	1.00	31.60
		ATOM	977	CD2	LEU	429	26.825	4.573	38.903	1.00	34.66
	10	ATOM	978	C	LEU	429	26.319	8.681	37.466	1.00	30.46
		ATOM	979	0	LEU	429	25.143	8.901	37.769	1.00	28.40
		MOTA	980	N	ALA	430	27.193	9.656	37.237	1.00	31.34
		MOTA	981	CA	ALA	430	26.806	11.059	37.332	1.00	29.83
		MOTA	982	CB	ALA	430	28.017	11.951	37.078	1.00	31.29
	15	ATOM	983	C	ALA	430	25.696	11.387	36.344	1.00	31.04
		ATOM	984	0	ALA	430	24.753	12.107	36.674	1.00	30.79
		ATOM	985	N	THR	431	25.802	10.854	35.128	1.00	30.30
		ATOM	986	CA	THR	431	24.786	11.105	34.112	1.00	28.81
		ATOM	987	CB	THR	431	25.207	10.533	32.737	1.00	30.55
	20	ATOM	988	OG1	THR	431	26.569	10.893	32.465	1.00	31.88
	20	ATOM	989	CG2	THR	431	24.321	11.087	31.634	1.00	25.63
		ATOM	990	C	THR	431	23.462	10.481	34.530	1.00	29.49
		ATOM	991	0	THR	431	22.402	11.099	34.397	1.00	26.18
						431	23.520	9.253	35.037	1.00	28.11
	25	MOTA	992	N	SER						
1	23	MOTA	993	CA	SER	432	22.308	8.573	35.480	1.00	29.78
40		ATOM	994	CB	SER	432	22.639	7.177	36.008	1.00	33.11
173		ATOM	995	OG	SER	432	21.454	6.412	36.136	1.00	36.92
10		ATOM	996	C	SER	432	21.651	9.399	36.589	1.00	31.49
Total		ATOM	997	0	SER	432	20.433	9.576	36.613	1.00	30.09
5,5	30	ATOM	998	N	ASER	433	22.476	9.901	37.496	0.75	32.09
- Jude		ATOM	999	N	BSER	433	22.474	9.906	37.500	0.25	31.10
h.		ATOM	1000	CA	ASER	433	22.002	10.715	38.605	0.75	35.68
16		ATOM	1001	CA	BSER	433	21.985	10.717	38.608	0.25	32.21
		ATOM	1002	CB	ASER	433	23.185	11.097	39.502	0.75	37.18
	35	MOTA	1003	CB	BSER	433	23.145	11.104	39.529	0.25	31.45
3434		MOTA	1004	OG	ASER	433	22.823	12.090	40.443	0.75	44.09
112		ATOM	1005	OG	BSER	433	23.785	9.953	40.053	0.25	29.52
deser		ATOM	1006	C	ASER	433	21.299	11.971	38.091	0.75	35.01
100		ATOM	1007	C	BSER	433	21.295	11.976	38.092	0.25	32.88
1113	40	ATOM	1008	0	ASER	433	20.257	12.373	38.612	0.75	35.34
		ATOM	1009	0	BSER	433	20.264	12.391	38.622	0.25	33.42
		ATOM	1010	N	ARG	434	21.867	12.579	37.054	1.00	33.38
		ATOM	1011	CA	ARG	434	21.300	13.788	36.470	1.00	34.19
		ATOM	1012	CB	ARG	434	22.239	14.354	35.400	1.00	33.89
	45	ATOM	1013	CG	ARG	434	21.670	15.528	34.625	1.00	38.30
		ATOM	1014	CD	ARG	434	21.559	16.787	35.479	1.00	37.91
		ATOM	1015	NE	ARG	434	21.158	17.944	34.680	1.00	37.78
		ATOM	1016	CZ	ARG	434	20.488	18.995	35.149	1.00	41.06
		ATOM	1017	NH1	ARG	434	20.132	19.049	36.428	1.00	40.70
	50	ATOM	1017	NH2	ARG	434	20.175	19.998	34.337	1.00	38.78
	50	ATOM	1018	C	ARG	434	19.937	13.491	35.873	1.00	33.48
											30.54
		ATOM	1020	0	ARG	434	18.996	14.266	36.053	1.00	
		ATOM	1021	N	PHE	435	19.831	12.371	35.158	1.00	34.68
	~ ~	ATOM	1022	CA	PHE	435	18.563	11.963	34.549	1.00	35.02
	55	ATOM	1023	CB	PHE	435	18.727	10.634	33.796	1.00	34.96
		ATOM	1024	CG	PHE	435	19.240	10.779	32.386	1.00	37.63
		ATOM	1025	CD1	PHE	435	19.459	12.035	31.824	1.00	42.03
		MOTA	1026	CD2	PHE	435	19.521	9.649	31.623	1.00	41.24
		MOTA	1027	CE1	PHE	435	19.953	12.164	30.521	1.00	43.11
	60	MOTA	1028	CE2	PHE	435	20.016	9.768	30.322	1.00	40.59
		MOTA	1029	CZ	PHE	435	20.233	11.029	29.775	1.00	40.63
		ATOM	1030	C	PHE	435	17.527	11.780	35.657	1.00	35.49

	5	ATOM	1031	0	PHE	435	16.361	12.135	35.496	1.00	34.78
		ATOM	1032	N	ARG	436	17.968	11.216	36.777	1.00	38.27
		ATOM	1033	CA	ARG	436	17.094	10.982	37.924	1.00	40.67
		ATOM	1034	CB	ARG	436	17.844	10.215	39.012	1.00	40.70
		ATOM	1035	CG	ARG	436	16.942	9.590	40.068	1.00	44.98
	10	ATOM		CD	ARG	436	17.648	8.459			
	10		1036						40.810	1.00	48.09
		ATOM	1037	NE	ARG	436	18.982	8.841	41.275	1.00	50.16
		ATOM	1038	CZ	ARG	436	20.119	8.361	40.777	1.00	52.19
		ATOM	1039	NH1	ARG	436	20.099	7.472	39.790	1.00	49.34
		ATOM	1040	NH2	ARG	436	21.283	8.770	41.266	1.00	51.85
	15	ATOM	1041	C	ARG	436	16.576	12.302	38.493	1.00	40.40
		ATOM	1042	0	ARG	436	15.382	12.458	38.730	1.00	41.49
		ATOM	1043	N	MET	437	17.477	13.252	38.706	1.00	40.02
		ATOM	1044	CA	MET	437	17.090	14.546	39.245	1.00	41.02
		ATOM	1045	CB	MET	437	18.329	15.427	39.440	1.00	40.29
	20	ATOM	1045	C	MET	437	16.099	15.221	38.299	1.00	40.23
	20		1045			437					
		ATOM		0	MET		15.111	15.805	38.734	1.00	42.46
		ATOM	1048	N	MET	438	16.367	15.127	37.001	1.00	39.02
		ATOM	1049	CA	MET	438	15.510	15.732	35.988	1.00	40.11
	~ ~	ATOM	1050	CB	MET	438	16.237	15.793	34.651	1.00	38.16
(2)	25	ATOM	1051	CG	MET	438	17.352	16.794	34.601	1.00	41.52
foreit of th		ATOM	1052	SD	MET	438	17.999	16.862	32.943	1.00	43.94
10		ATOM	1053	CE	MET	438	16.698	17.748	32.096	1.00	39.96
112		ATOM	1054	C	MET	438	14.221	14.964	35.783	1.00	37.72
10		ATOM	1055	0	MET	438	13.305	15.451	35.125	1.00	36.82
- ini	30	ATOM	1056	N	ASN	439	14.155	13.759	36.337	1.00	38.81
J		ATOM	1057	CA	ASN	439	12.981	12.919	36.174	1.00	40.77
ş <u>5</u>		ATOM	1058	CB	ASN	439	11.762	13.556	36.847	1.00	44.52
N		ATOM	1059	CG	ASN	439	10.566	12.620	36.887	1.00	48.29
6		ATOM	1060	OD1	ASN	439	10.721	11.400	36.964	1.00	48.48
(11)	35	ATOM	1061	ND2	ASN	439	9.365	13.189	36.829	1.00	50.23
1,4	33										
W		ATOM	1062	C	ASN	439	12.725	12.744	34.677	1.00	39.36
L)		MOTA	1063	0	ASN	439	11.637	13.037	34.172	1.00	37.76
150		ATOM	1064	N	LEU	440	13.749	12.274	33.972	1.00	37.65
100	40	MOTA	1065	CA	LEU	440	13.655	12.052	32.532	1.00	35.22
1000	40	ATOM	1066	CB	LEU	440	14.999	11.576	31.987	1.00	34.70
		ATOM	1067	CG	LEU	440	15.022	11.467	30.462	1.00	35.45
		ATOM	1068	CD1	LEU	440	14.890	12.862	29.869	1.00	35.24
		MOTA	1069	CD2	LEU	440	16.297	10.795	29.999	1.00	35.30
		MOTA	1070	C	LEU	440	12.587	11.024	32.196	1.00	36.48
	45	ATOM	1071	0	LEU	440	12.518	9.967	32.826	1.00	37.36
		ATOM	1072	N	GLN	441	11.763	11.328	31.197	1.00	36.82
		ATOM	1073	CA	GLN	441	10.696	10.420	30.785	1.00	38.51
		ATOM	1074	CB	GLN	441	9.431	11.211	30.443	1.00	38.23
		ATOM	1075	CG	GLN	441	8.912	12.063	31.592	1.00	42.46
	50	ATOM	1076	CD	GLN	441	8.362	11.227	32.729	1.00	44.91
	50	ATOM	1077	OE1	GLN	441	7.268	10.668	32.629	1.00	47.31
		ATOM	1078	NE2	GLN	441	9.119	11.132	33.818	1.00	44.06
		ATOM	1079	C	GLN	441	11.099	9.565	29.585	1.00	38.48
		MOTA	1080	0	GLN	441	11.923	9.976	28.763	1.00	35.80
	55	ATOM	1081	N	GLY	442	10.500	8.378	29.494	1.00	36.03
		ATOM	1082	CA	GLY	442	10.792	7.468	28.401	1.00	37.72
		ATOM	1083	C	GLY	442	10.599	8.112	27.043	1.00	36.88
		ATOM	1084	0	GLY	442	11.381	7.877	26.123	1.00	33.72
		ATOM	1085	N	GLU	443	9.556	8.925	26.918	1.00	36.59
	60	ATOM	1086	CA	GLU	443	9.269	9.603	25.661	1.00	37.13
		ATOM	1087	CB	GLU	443	7.956	10.379	25.764	1.00	41.57
		ATOM	1088	CG	GLU	443	6.723	9.488	25.879	1.00	47.76
							_	_	_		

	5	ATOM	1089	CD	GLU	443	6.483	9.008	27.302	1.00	53.96
		ATOM	1090	OE1	GLU	443	5.619	8.123	27.498	1.00	57.66
		ATOM	1091	OE2	GLU	443	7.159	9.515	28.225	1.00	56.13
		ATOM	1092	C	GLU	443	10.408	10.551	25.311	1.00	35.27
		ATOM	1093	ō	GLU	443	10.759	10.704	24.145	1.00	33.85
	10	ATOM	1094	N	GLU	444	10.984	11.179	26.331	1.00	32.09
	10		1095	CA	GLU	444		12.095	26.126	1.00	33.92
		ATOM					12.097				
		ATOM	1096	CB	GLU	444	12.332	12.924	27.388	1.00	34.97
		ATOM	1097	CG	GLU	444	11.169	13.845	27.732	1.00	38.28
		ATOM	1098	CD	GLU	444	11.383	14.610	29.023	1.00	38.11
	15	ATOM	1099	OE1	GLU	444	11.800	13.993	30.026	1.00	39.53
		ATOM	1100	OE2	GLU	444	11.132	15.834	29.036	1.00	40.77
		ATOM	1101	C	GLU	444	13.356	11.305	25.770	1.00	33.59
		ATOM	1102	0	GLU	444	14.085	11.670	24.842	1.00	33.35
		ATOM	1103	N	PHE	445	13.590	10.215	26.501	1.00	30.68
	20	ATOM	1104	CA	PHE	445	14.753	9.357	26.276	1.00	32.49
		ATOM	1105	CB	PHE	445	14.703	8.139	27.203	1.00	29.35
		ATOM	1106	CG	PHE	445	15.667	7.047	26.828	1.00	30.78
		ATOM	1107	CD1	PHE	445	17.036	7.201	27.030	1.00	28.25
		ATOM	1108	CD2	PHE	445	15.205	5.863	26.266	1.00	30.62
4535	25	ATOM	1109	CE1	PHE	445	17.933	6.195	26.675	1.00	28.67
0		ATOM	1110	CE2	PHE	445	16.095	4.848	25.908	1.00	31.37
123		ATOM	1111	CZ	PHE	445	17.460	5.015	26.113	1.00	30.37
17.		ATOM	1112	C	PHE	445	14.850	8.885	24.829	1.00	31.11
(0		ATOM	1113	ō	PHE	445	15.924	8.947	24.221	1.00	32.20
[mh	30	ATOM	1114	N	VAL	446	13.739	8.415	24.266	1.00	28.63
14	50	ATOM	1115	CA	VAL	446	13.787	7.943	22.889	1.00	27.94
į min		ATOM	1116	CB	VAL	446	12.478	7.193	22.478	1.00	28.48
14		ATOM	1117	CG1	VAL	446	12.318	5.939	23.343	1.00	29.61
5/		ATOM	1118	CG2	VAL	446	11.265	8.092	22.607	1.00	27.23
1.00	35										
1.3	33	ATOM	1119	C	VAL	446	14.099	9.064	21.900	1.00	27.28 28.07
1.0		MOTA	1120	0	VAL	446	14.781	8.837	20.904	1.00	
100		ATOM	1121	N	CYS	447	13.619	10.275	22.166	1.00	28.97
-65		ATOM	1122	CA	CYS	447	13.919	11.394	21.272	1.00	29.14
Ø	40	ATOM	1123	CB	CYS	447	13.156	12.653	21.693	1.00	28.90
1250	40	ATOM	1124	SG	CYS	447	11.389	12.591	21.309	1.00	35.68
		ATOM	1125	C	CYS	447	15.420	11.677	21.328	1.00	28.03
		ATOM	1126	0	CYS	447	16.063	11.885	20.302	1.00	29.34
		ATOM	1127	N	LEU	448	15.969	11.686	22.538	1.00	27.28
		ATOM	1128	CA	LEU	448	17.392	11.938	22.729	1.00	25.30
	45	ATOM	1129	CB	LEU	448	17.733	11.932	24.220	1.00	27.72
		ATOM	1130	CG	LEU	448	17.248	13.135	25.040	1.00	29.54
		ATOM	1131	CD1	LEU	448	17.807	13.042	26.454	1.00	30.85
		ATOM	1132	CD2	LEU	448	17.688	14.434	24.376	1.00	30.24
		MOTA	1133	C	LEU	448	18.245	10.902	22.008	1.00	27.62
	50	ATOM	1134	0	LEU	448	19.207	11.252	21.327	1.00	25.10
		ATOM	1135	N	LYS	449	17.905	9.621	22.162	1.00	25.16
		ATOM	1136	CA	LYS	449	18.673	8.570	21.506	1.00	27.55
		ATOM	1137	CB	LYS	449	18.135	7.185	21.900	1.00	28.99
		ATOM	1138	CG	LYS	449	19.134	6.052	21.694	1.00	34.70
	55	ATOM	1139	CD	LYS	449	18.737	4.789	22.459	1.00	32.67
		ATOM	1140	CE	LYS	449	17.267	4.419	22.220	1.00	31.87
		ATOM	1141	NZ	LYS	449	17.022	2.967	22.472	1.00	29.14
		ATOM	1142	C	LYS	449	18.626	8.749	19.990	1.00	25.88
		ATOM	1143	ō	LYS	449	19.610	8.489	19.296	1.00	25.93
	60	ATOM	1144	N	SER	450	17.482	9.197	19.480	1.00	26.07
	00	ATOM	1145	CA	SER	450	17.323	9.421	18.052	1.00	27.24
		ATOM	1145	CB	SER	450	15.857	9.705	17.721	1.00	32.24
		FILOR	T140	-	-	-200	13.037	2.703	-1.121	1.00	Ja.21

	5	ATOM	1263	CD1	LEU	466	22.156	18.002	-7.482	1.00	48.32
		ATOM	1264	CD2	LEU	466	22.033	18.594	-5.057	1.00	48.14
		ATOM	1265	C	LEU	466	23.817	16.397	-3.650	1.00	48.16
		ATOM	1266	0	LEU	466	22.961	16.845	-2.883	1.00	45.90
		ATOM	1267	N	LYS	467	24.093	15.099	-3.750	1.00	46.47
	10	ATOM	1268	CA	LYS	467	23.399	14.100	-2.947	1.00	47.45
		MOTA	1269	CB	LYS	467	23.802	12.693	-3.395	1.00	49.38
		ATOM	1270	CG	LYS	467	22.829	11.602	-2.974	1.00	52.70
		ATOM	1271	CD		467					
		ATOM	1271	CE	LYS	467	23.561	10.301	-2.682	1.00	56.48
	15			NZ	LYS		23.105	9.180	-3.604	1.00	59.54
	13	ATOM	1273		LYS	467	24.150	8.117	-3.732	1.00	61.22
		ATOM	1274	C	LYS	467	23.738	14.284	-1.472	1.00	46.89
		ATOM	1275	0	LYS	467	22.884	14.108	-0.604	1.00	46.06
		ATOM	1276	N	SER	468	24.989	14.644	-1.202	1.00	45.82
	20	ATOM	1277	CA	SER	468	25.457	14.854	0.160	1.00	46.82
	20	MOTA	1278	CB	SER	468	26.976	15.050	0.173	1.00	47.85
		ATOM	1279	OG	SER	468	27.407	15.537	1.435	1.00	55.73
		MOTA	1280	C	SER	468	24.778	16.063	0.790	1.00	44.24
		MOTA	1281	0	SER	468	24.473	16.062	1.983	1.00	42.98
		ATOM	1282	N	LEU	469	24.547	17.100	-0.011	1.00	42.33
green.	25	ATOM	1283	CA	LEU	469	23.890	18.301	0.486	1.00	40.42
		MOTA	1284	CB	LEU	469	24.002	19.427	-0.545	1.00	44.47
111		MOTA	1285	CG	LEU	469	25.438	19.874	-0.849	1.00	46.70
10		MOTA	1286	CD1	LEU	469	25.514	20.477	-2.246	1.00	46.70
lyst.		MOTA	1287	CD2	LEU	469	25.890	20.883	0.199	1.00	47.32
14	30	ATOM	1288	C	LEU	469	22.423	17.996	0.786	1.00	39.06
		MOTA	1289	0	LEU	469	21.856	18.505	1.760	1.00	34.97
Esche.		ATOM	1290	N	GLU	470	21.814	17.151	-0.046	1.00	35.46
1		MOTA	1291	CA	GLU	470	20.418	16.768	0.145	1.00	34.38
21		ATOM	1292	CB	GLU	470	19.914	15.963	-1.052	1.00	38.02
55 122 143	35	ATOM	1293	CG	GLU	470	19.772	16.773	-2.329	1.00	42.67
100		ATOM	1294	CD	GLU	470	19.339	15.923	-3.509	1.00	48.30
Į.J		ATOM	1295	OE1	GLU	470	19.671	14.716	-3.538	1.00	50.53
(2)		ATOM	1296	OE2	GLU	470	18.666	16.463	-4.412	1.00	51.06
+G		ATOM	1297	C	GLU	470	20.290	15.916	1.403	1.00	34.37
1	40	ATOM	1298	Ō	GLU	470	19.321	16.035	2.157	1.00	32.60
		ATOM	1299	N	GLU	471	21.274	15.046	1.606	1.00	34.66
		ATOM	1300	CA	GLU	471	21.309	14.162	2.766	1.00	35.68
		ATOM	1301	CB	GLU	471	22.515	13.222	2.671	1.00	34.57
		ATOM	1302	CG	GLU	471	22.376	12.122	1.614	1.00	37.98
	45	ATOM	1302	CD	GLU	471	21.476	10.989	2.063	1.00	39.79
	••	ATOM	1304	OE1	GLU	471	20.268	11.027	1.743	1.00	41.12
		ATOM	1305	OE2	GLU	471	21.974	10.061	2.737	1.00	32.11
		ATOM	1306	C	GLU	471	21.393	14.983	4.052	1.00	34.79
		ATOM	1307	0	GLU	471		14.793		1.00	
	50	ATOM	1307	N	LYS	472	20.596 22.358	15.898	4.969 4.112		32.80 33.93
	50			CA		472				1.00	
		MOTA	1309		LYS		22.518	16.739	5.291	1.00	35.58
		ATOM	1310	CB	LYS	472	23.683	17.710	5.097	1.00	39.11
		ATOM	1311	CG	LYS	472	25.050	17.050	5.138	1.00	41.47
		ATOM	1312	CD	LYS	472	26.080	17.957	5.794	1.00	46.97
	55	ATOM	1313	CE	LYS	472	27.445	17.286	5.862	1.00	48.40
		ATOM	1314	NZ	LYS	472	27.850	16.702	4.547	1.00	51.55
		MOTA	1315	C	LYS	472	21.237	17.523	5.582	1.00	34.78
		ATOM	1316	0	LYS	472	20.795	17.607	6.724	1.00	33.95
	c0	ATOM	1317	N	ASP	473	20.643	18.097	4.545	1.00	33.47
	60	ATOM	1318	CA	ASP	473	19.420	18.865	4.720	1.00	34.63
		ATOM	1319	CB	ASP	473	18.923	19.404	3.380	1.00	37.21
		ATOM	1320	CG	ASP	473	17.654	20.221	3.522	1.00	43.24

	5	ATOM	1321	OD1	ASP	473	16.559	19.687	3.230	1.00	45.20
		ATOM	1322	OD2	ASP	473	17.750	21.396	3.932	1.00	45.59
		ATOM	1323	C	ASP	473	18.339	17.998	5.338	1.00	32.93
		ATOM	1324	0	ASP	473	17.642	18.416	6.264	1.00	32.87
		ATOM	1325	N	HIS	474	18.199	16.784	4.827		
	10									1.00	32.74
	10	ATOM	1326	CA	HIS	474	17.185	15.882	5.343	1.00	32.21
		ATOM	1327	CB	HIS	474	17.185	14.575	4.568	1.00	32.79
		ATOM	1328	CG	HIS	474	16.047	13.675	4.924	1.00	36.22
		ATOM	1329	CD2	HIS	474	14.711	13.813	4.750	1.00	38.33
		ATOM	1330	ND1	HIS	474	16.227	12.456	5.542	1.00	38.97
	15	ATOM	1331	CE1	HIS	474	15.053	11.883	5.732	1.00	37.99
		ATOM	1332	NE2	HIS	474	14.116	12.686	5.261	1.00	37.43
		ATOM	1333	C	HIS	474	17.403	15.573	6.815	1.00	29.74
		ATOM	1334	ō	HIS	474	16.460	15.543	7.596	1.00	29.90
		ATOM	1335	N	ILE	475	18.653	15.326	7.185	1.00	
	20	ATOM		CA		475					27.80
	20		1336		ILE		18.971	15.014	8.571	1.00	25.61
		ATOM	1337	CB	ILE	475	20.478	14.708	8.720	1.00	25.59
		ATOM	1338	CG2	ILE	475	20.877	14.713	10.193	1.00	27.17
		ATOM	1339	CG1	ILE	475	20.787	13.341	8.092	1.00	26.17
		ATOM	1340	CD1	ILE	475	22.258	13.071	7.849	1.00	27.07
100	25	ATOM	1341	C	ILE	475	18.576	16.201	9.460	1.00	27.91
trad do		ATOM	1342	0	ILE	475	17.928	16.038	10.485	1.00	29.16
10		ATOM	1343	N	HIS	476	18.956	17.404	9.054	1.00	29.41
10		ATOM	1344	CA	HIS	476	18.621	18.575	9.846	1.00	29.73
(1)		ATOM	1345	CB	HIS	476	19.342	19.796	9.281	1.00	32.27
1.4	30	ATOM	1346	CG	HIS	476	20.777	19.867	9.699	1.00	39.44
74.3		ATOM	1347	CD2	HIS	476	21.355	19.707	10.915		
1.5		ATOM	1348	ND1	HIS	476	21.809	20.067	8.808	1.00	39.81
14		ATOM	1349	CE1						1.00	39.79
6					HIS	476	22.959	20.027	9.456	1.00	39.98
land.	35	ATOM	1350	NE2	HIS	476	22.712	19.809	10.735	1.00	40.26
145	33	ATOM	1351	C	HIS	476	17.120	18.810	9.948	1.00	31.40
1.1		ATOM	1352	0	HIS	476	16.636	19.336	10.951	1.00	29.79
11		MOTA	1353	N	ARG	477	16.374	18.396	8.929	1.00	31.82
7100		ATOM	1354	CA	ARG	477	14.929	18.570	8.956	1.00	31.53
40		ATOM	1355	CB	ARG	477	14.343	18.376	7.557	1.00	34.95
110	40	MOTA	1356	CG	ARG	477	14.425	19.627	6.700	1.00	40.46
		ATOM	1357	CD	ARG	477	13.698	19.445	5.370	1.00	45.22
		MOTA	1358	NE	ARG	477	14.107	20.456	4.399	1.00	53.05
		ATOM	1359	CZ	ARG	477	13.647	21.705	4.376	1.00	55.89
		MOTA	1360	NH1	ARG	477	12.756	22.106	5.274	1.00	56.17
	45	ATOM	1361	NH2	ARG	477	14.084	22.558	3.457	1.00	59.49
		ATOM	1362	C	ARG	477	14.310	17.582	9.931	1.00	30.70
		ATOM	1363	0	ARG	477	13.360	17.903	10.649	1.00	30.24
		ATOM	1364	N	VAL	478	14.863	16.375	9.972	1.00	29.67
		ATOM	1365	CA	VAL	478	14.351				
	50							15.369	10.887	1.00	29.68
	30	ATOM	1366	CB	VAL	478	14.937	13.975	10.575	1.00	32.01
		ATOM	1367	CG1	VAL	478	14.461	12.973	11.609	1.00	32.93
		ATOM	1368	CG2	VAL	478	14.506	13.528	9.169	1.00	31.00
		ATOM	1369	C	VAL	478	14.696	15.774	12.316	1.00	29.81
		ATOM	1370	0	VAL	478	13.860	15.677	13.220	1.00	30.25
	55	ATOM	1371	N	LEU	479	15.929	16.232	12.516	1.00	28.81
		ATOM	1372	CA	LEU	479	16.360	16.674	13.836	1.00	28.74
		ATOM	1373	CB	LEU	479	17.799	17.210	13.779	1.00	26.65
		ATOM	1374	CG	LEU	479	18.910	16.152	13.853	1.00	26.05
		ATOM	1375	CD1	LEU	479	20.231	16.772	13.395	1.00	25.81
	60	ATOM	1376	CD2	LEU	479	19.028	15.603	15.277	1.00	25.34
		ATOM	1377	C	LEU	479	15.411	17.777	14.313	1.00	29.54
		ATOM	1378	0	LEU	479	14.997	17.786	15.472	1.00	29.00
		FILORI	10/0	9	2150	415	14.22/	17.700	13.4/2	1.00	29.00

	5	ATOM	1379	N	ASP	480	15.076	18.703	13.415	1.00	31.52
		ATOM	1380	CA	ASP	480	14.162	19.800	13.741	1.00	33.84
		ATOM	1381	CB	ASP	480	13.943	20.712	12.528	1.00	34.37
		ATOM	1382	CG	ASP	480	15.055	21.743	12.345	1.00	36.26
	10	ATOM	1383	OD1	ASP	480	15.119	22.354	11.257	1.00	36.56
	10	MOTA	1384	OD2	ASP	480	15.860	21.951	13.274	1.00	34.19
		ATOM	1385	C	ASP	480	12.818	19.222	14.174	1.00	33.48
		MOTA	1386	0	ASP	480	12.186	19.724	15.105	1.00	33.89
		ATOM	1387	N	LYS	481	12.379	18.161	13.498	1.00	33.90
		ATOM	1388	CA	LYS	481	11.106	17.536	13.839	1.00	32.97
	15	ATOM	1389	CB	LYS	481	10.719	16.489	12.784	1.00	34.66
	15	ATOM	1390	C	LYS	481	11.164	16.895	15.225	1.00	33.57
		ATOM	1391	0	LYS	481	10.167	16.869	15.943	1.00	35.37
		ATOM	1392	N	ILE	482	12.328	16.377	15.607	1.00	32.71
		ATOM	1393	CA	ILE	482	12.457	15.764	16.922	1.00	31.60
	20	MOTA	1394	CB	ILE	482	13.743	14.913	17.028	1.00	32.65
		ATOM	1395	CG2	ILE	482	13.877	14.338	18.430	1.00	32.50
		ATOM	1396	CG1	ILE	482	13.697	13.785	15.995	1.00	32.72
		ATOM	1397	CD1	ILE	482	14.978	12.969	15.908	1.00	33.37
		ATOM	1398	C	ILE	482	12.456	16.853	17.994	1.00	31.69
	25	ATOM	1399	0	ILE	482	11.946	16.649	19.097	1.00	29.98
122	23										
10		ATOM	1400	N	THR	483	13.027	18.012	17.679	1.00	31.33
141		ATOM	1401	CA	THR	483	13.022	19.109	18.644	1.00	31.71
(7)		ATOM	1402	CB	THR	483	13.756	20.351	18.109	1.00	32.92
- India		ATOM	1403	OG1	THR	483	15.111	20.012	17.788	1.00	29.99
14	30	ATOM	1404	CG2	THR	483	13.756	21.452	19.160	1.00	30.47
1.4		ATOM	1405	C	THR	483	11.559	19.483	18.920	1.00	32.85
		ATOM	1406	0	THR	483	11.146	19.598	20.070	1.00	31.83
1248		ATOM	1407	N	ASP	484	10.785	19.656	17.851	1.00	31.91
6		ATOM	1408	CA	ASP	484	9.369	20.003	17.965	1.00	34.15
1,2	35	ATOM	1409	CB	ASP	484	8.708	20.003	16.591	1.00	37.41
L.J	55										
141		ATOM	1410	CG	ASP	484	9.270	21.080	15.680	1.00	42.02
7506 7400		ATOM	1411	OD1	ASP	484	9.871	22.045	16.198	1.00	43.26
10		ATOM	1412	OD2	ASP	484	9.106	20.952	14.445	1.00	42.49
4173		ATOM	1413	C	ASP	484	8.657	18.985	18.840	1.00	33.16
102.2	40	ATOM	1414	0	ASP	484	7.830	19.339	19.676	1.00	34.86
		ATOM	1415	N	THR	485	8.996	17.715	18.646	1.00	33.91
		ATOM	1416	CA	THR	485	8.396	16.635	19.414	1.00	34.41
		ATOM	1417	CB	THR	485	8.875	15.268	18.885	1.00	33.58
		ATOM	1418	OG1	THR	485	8.400	15.094	17.542	1.00	37.04
	45	ATOM	1419	CG2	THR	485	8.347	14.138	19.751	1.00	30.89
		ATOM	1420	C	THR	485	8.708	16.757	20.903	1.00	35.15
		ATOM	1421	0	THR	485	7.818	16.600	21.744	1.00	31.99
		ATOM	1422	N	LEU	486	9.966	17.046	21.229	1.00	33.77
		MOTA	1423	CA	LEU	486	10.368	17.192	22.621	1.00	34.31
	50	ATOM	1424	CB	LEU	486	11.879	17.448	22.721	1.00	32.00
		ATOM	1425	CG	LEU	486	12.776	16.201	22.754	1.00	34.99
		ATOM	1426	CD1	LEU	486	14.233	16.613	22.521	1.00	32.65
		ATOM	1427	CD2	LEU	486	12.635	15.481	24.105	1.00	29.90
		ATOM	1428	C	LEU	486	9.597	18.348	23.256	1.00	34.87
	55	ATOM	1429	Ö	LEU	486	9.078	18.225	24.362	1.00	35.85
	55	ATOM	1430	N	ILE	487	9.513	19.469	22.548	1.00	35.59
		ATOM	1431	CA	ILE	487	8.787	20.625	23.064	1.00	36.79
		ATOM	1432	CB	ILE	487	8.890	21.826	22.095	1.00	37.32
		ATOM	1433	CG2	ILE	487	7.833	22.884	22.443	1.00	40.19
	60	MOTA	1434	CG1	ILE	487	10.292	22.443	22.181	1.00	36.00
		ATOM	1435	CD1	ILE	487	10.635	23.041	23.544	1.00	33.58
		ATOM	1436	C	ILE	487	7.315	20.257	23.276	1.00	38.56

	5	ATOM	1437	0	ILE	487	6.708	20.628	24.282	1.00	38.52
		ATOM	1438	N	HIS	488	6.749	19.521	22.326	1.00	40.33
		ATOM	1439	CA	HIS	488	5.357	19.096	22.427	1.00	42.29
		ATOM	1440	CB	HIS	488	4.962	18.282	21.197	1.00	44.26
		ATOM	1441	CG	HIS	488	3.612	17.647	21.305	1.00	47.75
	10	ATOM	1442	CD2	HIS	488	2.369	18.175	21.214	1.00	47.46
		ATOM	1443	ND1	HIS	488	3.440	16.298	21.534	1.00	51.09
		ATOM	1444	CE1	HIS	488	2.148	16.023	21.577	1.00	51.15
		ATOM	1445	NE2	HIS	488	1.477	17.144	21.385	1.00	50.22
		ATOM	1446	C	HIS	488	5.154	18.254	23.685	1.00	42.55
	15	ATOM	1447	0	HIS	488	4.233	18.498	24.467		43.02
	13	ATOM	1448	N	LEU	489	6.022	17.266	23.879	1.00	
		ATOM	1449	CA	LEU	489	5.936			1.00	39.91
								16.399	25.048	1.00	39.93
		ATOM	1450	CB	LEU	489	7.087	15.396	25.048	1.00	38.83
	20	ATOM	1451	CG	LEU	489	6.961	14.242	24.056	1.00	39.31
	20	ATOM	1452	CD1	LEU	489	8.259	13.456	24.027	1.00	39.01
		ATOM	1453	CD2	LEU	489	5.799	13.345	24.459	1.00	41.98
		ATOM	1454	C	LEU	489	5.973	17.203	26.339	1.00	40.24
		ATOM	1455	0	LEU	489	5.267	16.888	27.298	1.00	38.72
	25	ATOM	1456	N	MET	490	6.798	18.246	26.353	1.00	39.94
Pota See	23	MOTA	1457	CA	MET	490	6.939	19.102	27.522	1.00	41.50
D N		MOTA	1458	CB	MET	490	8.208	19.953	27.394	1.00	39.15
[1]		MOTA	1459	CG	MET	490	9.495	19.169	27.608	1.00	41.69
(1)		MOTA	1460	SD	MET	490	10.978	20.106	27.161	1.00	35.76
1.25	30	MOTA	1461	CE	MET	490	12.178	18.775	27.056	1.00	39.22
14	30	ATOM	1462	C	MET	490	5.718	20.004	27.717	1.00	42.33
1.4		MOTA	1463	0	MET	490	5.296	20.258	28.848	1.00	41.09
4.1		MOTA	1464	N	ALA	491	5.162	20.498	26.616	1.00	43.15
23		MOTA	1465	CA	ALA	491	3.983	21.351	26.693	1.00	43.79
900	35	ATOM	1466	CB	ALA	491	3.622	21.879	25.311	1.00	43.93
3.0	33	MOTA	1467	C	ALA	491	2.841	20.510	27.251	1.00	46.16
100		ATOM	1468	O N	ALA	491	2.073	20.967	28.095	1.00	44.69
nor.		ATOM ATOM	1469 1470	CA	LYS LYS	492 492	2.752 1.711	19.268	26.783	1.00	46.29
15		ATOM	1471	CB	LYS	492		18.351	27.222	1.00	49.90
10	40	ATOM	1471	CG	LYS	492	1.772	17.053	26.411	1.00	50.03
. 3 404	70	ATOM	1473	CD	LYS	492	-0.002	17.135	25.062	1.00	53.81
		ATOM	1474	CE	LYS	492		16.084	24.930	1.00	59.00
		ATOM	1475	NZ	LYS	492	-0.988 -1.351	16.453 15.281	23.827 22.976	1.00	61.85
		ATOM	1476	C	LYS	492	1.841	18.025	28.701	1.00	62.89
	45	ATOM	1477	0	LYS	492	0.845	17.784	29.379	1.00	51.15 53.37
	45	ATOM	1478	N	ALA	493	3.072	18.012	29.199	1.00	50.15
		ATOM	1479	CA	ALA	493	3.321	17.706	30.600	1.00	49.17
		ATOM	1480	CB	ALA	493	4.777	17.314	30.794	1.00	50.39
		ATOM	1481	C	ALA	493	2.971	18.885	31.501	1.00	49.36
	50	ATOM	1482	0	ALA	493	3.089	18.799	32.723	1.00	51.57
	20	ATOM	1483	N	GLY	494	2.554	19.989	30.893	1.00	48.61
		ATOM	1484	CA	GLY	494	2.185	21.159	31.671	1.00	46.92
		ATOM	1485	C	GLY	494	3.322	22.107	32.006	1.00	45.46
		ATOM	1486	0	GLY	494	3.206	22.107	32.000	1.00	43.48
	55	ATOM	1487	N	LEU	495	4.431	22.009	31.284	1.00	44.81
	55	ATOM	1488	CA	LEU	495	5.555	22.899	31.540	1.00	42.34
		ATOM	1489	CB	LEU	495	6.847	22.293			
		ATOM	1490	CG	LEU	495	7.712	22.293	30.988 31.936	1.00	43.79
		ATOM	1490	CD1	LEU	495	7.712	20.156	32.260	1.00	40.99
	60	ATOM	1491	CD1	LEU	495	9.072	21.189	32.260	1.00	44.70
	50	ATOM	1492	CD2	LEU	495	5.278	24.227	30.847	1.00	42.12
		ATOM	1494	0	LEU	495	4.664	24.227	29.778	1.00	42.13
			1101	_		100	1.004	24.250	20.770	2.00	.2.23

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	5	ATOM	1495	N	THR	496	5.718	25.324	31.452	1.00	42.73
		ATOM	1496	CA	THR	496	5.521	26.636	30.845	1.00	43.56
		ATOM	1497	CB	THR	496	5.841	27.767	31.829	1.00	46.09
		ATOM	1498	OG1	THR	496	7.222	27.688	32.208	1.00	43.92
		ATOM	1499	CG2	THR	496	4.965	27.662	33.064	1.00	45.63
	10	ATOM	1500	C	THR	496	6.471	26.764	29.660	1.00	45.54
		ATOM	1501	0	THR	496	7.370	25.939	29.488	1.00	43.39
		ATOM	1502	N	LEU	497	6.280	27.800	28.849	1.00	45.02
		MOTA	1503	CA	LEU	497	7.135	28.020	27.688	1.00	45.12
		ATOM	1504	CB	LEU	497	6.710	29.286	26.944	1.00	46.62
	15	MOTA	1505	CG	LEU	497	5.933	29.080	25.640	1.00	50.20
		MOTA	1506	CD1	LEU	497	5.886	30.397	24.875	1.00	50.95
		MOTA	1507	CD2	LEU	497	6.589	27.990	24.798	1.00	50.91
		MOTA	1508	C	LEU	497	8.599	28.135	28.101	1.00	44.94
	20	MOTA	1509	0	LEU	497	9.474	27.516	27.493	1.00	45.03
	20	ATOM	1510	N	GLN	498	8.862	28.927	29.137	1.00	41.14
		MOTA	1511	CA	GLN	498	10.221	29.101	29.627	1.00	40.54
		MOTA	1512	CB	GLN	498	10.246	30.140	30.743	1.00	43.82
		MOTA	1513	CG	GLN	498	11.585	30.270	31.437	1.00	43.37
	25	ATOM	1514	CD	GLN	498	11.539	31.260	32.584	1.00	47.03
(2)	25	ATOM	1515	OE1	GLN	498	10.565	31.308	33.332	1.00	49.18
·D		ATOM	1516	NE2	GLN	498	12.591	32.054	32.727	1.00	45.30
11,5		ATOM	1517	C	GLN GLN	498 498	10.777 11.923	27.773 27.422	30.145	1.00	39.39
10		ATOM ATOM	1518 1519	O N	GLN	499	9.965	27.422	29.866 30.902	1.00	35.05 36.49
frah.	30	ATOM	1520	CA	GLN	499	10.391	25.748	31.434	1.00	36.49
100	50	ATOM	1521	CB	GLN	499	9.314	25.155	32.344	1.00	38.84
\$ well		ATOM	1522	CG	GLN	499	9.155	25.825	33.703	1.00	41.33
1		ATOM	1523	CD	GLN	499	8.039	25.187	34.512	1.00	42.74
21		ATOM	1524	OE1	GLN	499	7.027	24.760	33.955	1.00	45.44
114	35	ATOM	1525	NE2	GLN	499	8.222	25.107	35.829	1.00	43.48
ĮĮ.		ATOM	1526	C	GLN	499	10.655	24.773	30.285	1.00	35.03
1,0		ATOM	1527	0	GLN	499	11.446	23.832	30.422	1.00	36.59
125		ATOM	1528	N	GLN	500	9.980	24.994	29.162	1.00	34.14
× (2)		MOTA	1529	CA	GLN	500	10.136	24.138	27.990	1.00	34.65
1	40	ATOM	1530	CB	GLN	500	9.042	24.436	26.958	1.00	33.90
		MOTA	1531	CG	GLN	500	7.672	23.872	27.315	1.00	36.62
		MOTA	1532	CD	GLN	500	6.558	24.419	26.435	1.00	40.17
		MOTA	1533	OE1	GLN	500	6.660	24.417	25.207	1.00	40.22
		MOTA	1534	NE2	GLN	500	5.482	24.886	27.064	1.00	41.82
	45	ATOM	1535	C	GLN	500	11.511	24.350	27.358	1.00	34.96
		ATOM	1536	0	GLN	500	12.256	23.387	27.124	1.00	30.79
		MOTA	1537	N	HIS	501	11.835	25.612	27.078	1.00	34.21
		ATOM	1538	CA	HIS	501	13.117	25.966	26.480	1.00	37.42
		ATOM	1539	CB	HIS	501	13.195	27.476	26.246	1.00	43.08
	50	ATOM	1540	CG	HIS	501	12.043	28.027	25.468	1.00	51.13
		ATOM	1541	CD2	HIS	501	11.534	27.678	24.263	1.00	53.05
		ATOM	1542	ND1	HIS	501	11.264	29.068	25.926	1.00	54.54
		ATOM	1543 1544	CE1 NE2	HIS HIS	501 501	10.325	29.337	25.037	1.00	54.36 55.19
	55	ATOM ATOM	1544	C	HIS	501	10.466 14.255	28.508 25.543	24.018 27.395	1.00	35.79
	33	ATOM	1546	0	HIS	501	15.271	24.996	26.945	1.00	36.20
		ATOM	1546	N	GLN	502	14.086	25.799	28.685	1.00	38.20
		ATOM	1548	CA	GLN	502	15.110	25.438	29.650	1.00	32.18
		ATOM	1549	CB	GLN	502	14.740	25.977	31.033	1.00	35.84
	60	ATOM	1550	CG	GLN	502	14.787	27.498	31.113	1.00	32.66
	-	ATOM	1551	CD	GLN	502	14.420	28.028	32.486	1.00	36.62
		ATOM	1552	OE1	GLN	502	14.102	27.262	33.397	1.00	33.99
							249				
							247				

	5	ATOM	1553	NE2	GLN	502	14.462	29.348	32.640	1.00	36.22
		MOTA	1554	C	GLN	502	15.340	23.932	29.716	1.00	31.79
		ATOM	1555	0	GLN	502	16.483	23.479	29.769	1.00	28.00
		MOTA	1556	N	ARG	503	14.266	23.146	29.705	1.00	30.99
		ATOM	1557	CA	ARG	503	14.436	21.704	29.779	1.00	29.91
	10	ATOM	1558	CB	ARG	503	13.107	21.011	30.052	1.00	32.79
		MOTA	1559	CG	ARG	503	13.258	19.541	30.400	1.00	30.84
		ATOM	1560	CD	ARG	503	11.930	18.935	30.798	1.00	30.61
		ATOM	1561	NE	ARG	503	12.021	17.490	30.992	1.00	28.50
		ATOM	1562	CZ	ARG	503	12.489	16.908	32.093	1.00	29.00
	15	MOTA	1563	NH1	ARG	503	12.917	17.640	33.114	1.00	29.85
		ATOM	1564	NH2	ARG	503	12.512	15.583	32.180	1.00	33.73
		ATOM	1565	C	ARG	503	15.051	21.152	28.496	1.00	29.89
		MOTA	1566	0	ARG	503	15.895	20.259	28.548	1.00	29.69
		ATOM	1567	N	LEU	504	14.624	21.675	27.351	1.00	28.99
	20	ATOM	1568	CA	LEU	504	15.164	21.223	26.075	1.00	28.90
		ATOM	1569	CB	LEU	504	14.566	22.023	24.916	1.00	27.72
		ATOM	1570	CG	LEU	504	15.327	21.901	23.593	1.00	30.47
		ATOM	1571	CD1	LEU	504	15.252	20.453	23.117	1.00	31.74
		ATOM	1572	CD2	LEU	504	14.742	22.843	22.542	1.00	29.85
2094	25	ATOM	1573	C	LEU	504	16.681	21.419	26.089	1.00	29.69
		ATOM	1574	0	LEU	504	17.439	20.536	25.672	1.00	26.38
10		ATOM	1575	N	ALA	505	17.114	22.585	26.564	1.00	28.51
		ATOM	1576	CA	ALA	505	18.535	22.899	26.632	1.00	25.98
10		MOTA	1577	CB	ALA	505	18.735	24.361	27.039	1.00	29.86
neb 1	30	MOTA	1578	C	ALA	505	19.261	21.977	27.604	1.00	26.67
H		ATOM	1579	0	ALA	505	20.340	21.462	27.290	1.00	25.54
grafe 4		ATOM	1580	N	GLN	506	18.677	21.771	28.784	1.00	23.59
1-4		ATOM	1581	CA	GLN	506	19.299	20.907	29.785	1.00	27.67
21		ATOM	1582	CB	GLN	506	18.434	20.796	31.043	1.00	27.75
1585	35	ATOM	1583	CG	GLN	506	18.414	22.027	31.945	1.00	32.48
W		ATOM	1584	CD	GLN	506	17.111	22.116	32.736	1.00	38.40
14		ATOM	1585	OE1	GLN	506	16.319	21.167	32.754	1.00	35.97
1195		ATOM	1586	NE2	GLN	506	16.879	23.257	33.386	1.00	38.07
4.0		ATOM	1587	C	GLN	506	19.500	19.509	29.217	1.00	24.53
1	40	ATOM	1588	0	GLN	506	20.536	18.889	29.441	1.00	26.42
		ATOM	1589	N	LEU	507	18.505	19.017	28.484	1.00	26.78
		ATOM	1590	CA	LEU	507	18.578	17.678	27.902	1.00	26.18
		ATOM	1591	CB	LEU	507	17.225	17.286	27.295	1.00	31.48
		ATOM	1592	CG	LEU	507	16.052	16.961	28.231	1.00	32.59
	45	ATOM	1593	CD1	LEU	507	14.836	16.561	27.389	1.00	33.78
		ATOM	1594	CD2	LEU	507	16.431	15.838	29.174	1.00	30.18
		ATOM	1595	C	LEU	507	19.652	17.583	26.819	1.00	26.03
		MOTA	1596	0	LEU	507	20.421	16.621	26.771	1.00	27.28
		ATOM	1597	N	LEU	508	19.713	18.583	25.950	1.00	24.31
	50	ATOM	1598	CA	LEU	508	20.690	18.557	24.863	1.00	23.68
		ATOM	1599	CB	LEU	508	20.339	19.629	23.828	1.00	23.91
		ATOM	1600	CG	LEU	508	19.004	19.436	23.102	1.00	24.68
		MOTA	1601	CD1	LEU	508	18.905	20.416	21.945	1.00	25.11
		MOTA	1602	CD2	LEU	508	18.903	17.994	22.580	1.00	27.53
	55	ATOM	1603	C	LEU	508	22.127	18.727	25.341	1.00	22.93
		ATOM	1604	0	LEU	508	23.062	18.200	24.736	1.00	21.36
		ATOM	1605	N	LEU	509	22.302	19.451	26.441	1.00	23.86
		ATOM	1606	CA	LEU	509	23.637	19.661	26.991	1.00	26.28
		ATOM	1607	CB	LEU	509	23.598	20.735	28.095	1.00	28.08
	60	MOTA	1608	CG	LEU	509	23.578	22.214	27.672	1.00	33.98
		ATOM	1609	CD1	LEU	509	23.529	23.114	28.921	1.00	35.23
		MOTA	1610	CD2	LEU	509	24.818	22.525	26.856	1.00	30.48

	5	ATOM	1611	C	LEU	509	24.154	18.327	27.540	1.00	26.08
		ATOM	1612	0	LEU	509	25.354	18.068	27.547	1.00	23.92
		MOTA	1613	N	ILE	510	23.254	17.462	27.993	1.00	24.60
		ATOM	1614	CA	ILE	510	23.712	16.172	28.496	1.00	25.12
		MOTA	1615	CB	ILE	510	22.568	15.368	29.161	1.00	28.51
	10	ATOM	1616	CG2	ILE	510	23.051	13.965	29.506	1.00	31.67
		ATOM	1617	CG1	ILE	510	22.141	16.060	30.459	1.00	31.18
		ATOM	1618	CD1	ILE	510	20.712	15.749	30.882	1.00	37.16
		ATOM	1619	CDI	ILE	510	24.337	15.749	27.364	1.00	23.86
									27.600		
	15	ATOM	1620	0	ILE	510	25.225	14.534		1.00	24.14
	13	ATOM	1621	N	LEU	511	23.889	15.586	26.133	1.00	25.10
		ATOM	1622	CA	LEU	511	24.420	14.862	24.977	1.00	25.63
		ATOM	1623	CB	LEU	511	23.628	15.225	23.714	1.00	23.89
		ATOM	1624	CG	LEU	511	22.152	14.801	23.659	1.00	25.78
		MOTA	1625	CD1	LEU	511	21.648	14.920	22.224	1.00	26.55
	20	ATOM	1626	CD2	LEU	511	21.990	13.363	24.146	1.00	26.29
		ATOM	1627	C	LEU	511	25.912	15.152	24.771	1.00	27.10
		ATOM	1628	0	LEU	511	26.641	14.332	24.214	1.00	24.98
		MOTA	1629	N	SER	512	26.372	16.319	25.213	1.00	24.75
		MOTA	1630	CA	SER	512	27.787	16.637	25.076	1.00	23.68
4000	25	MOTA	1631	CB	SER	512	28.023	18.129	25.358	1.00	26.12
100		ATOM	1632	OG	SER	512	29.271	18.327	25.986	1.00	37.17
403		ATOM	1633	C	SER	512	28.594	15.765	26.050	1.00	23.15
IU		ATOM	1634	0	SER	512	29.742	15.383	25.769	1.00	22.15
40		ATOM	1635	N	AHIS	513	27.993	15.456	27.192	0.50	21.53
- de	30	ATOM	1636	N	BHIS	513	28.008	15.453	27.202	0.50	20.99
1		ATOM	1637	CA	AHIS	513	28.645	14.624	28.196	0.50	21.79
ž sk		ATOM	1638	CA	BHIS	513	28.696	14.607	28.174	0.50	20.94
14		ATOM	1639	CB	AHIS	513	27.920	14.776	29.536	0.50	23.59
21		ATOM	1640	CB	BHIS	513	27.991	14.636	29.536	0.50	21.59
100	35	ATOM	1641	CG	AHIS	513	28.145	16.109	30.179	0.50	27.34
L.J		ATOM	1642	CG	BHIS	513	28.800	14.032	30.642	0.50	23.94
luj.		ATOM	1643	CD2	AHIS	513	29.223	16.616	30.824	0.50	27.56
4100 F100		ATOM	1644	CD2	BHIS	513	30.095	14.211	31.001	0.50	24.22
40		ATOM	1645	ND1	AHIS	513	27.204	17.117	30.160	0.50	30.62
4.13	40	ATOM	1646	ND1	BHIS	513	28.285	13.105	31.523	0.50	27.00
		ATOM	1647	CE1	AHIS	513	27.693	18.185	30.763	0.50	26.32
		ATOM	1648	CE1	BHIS	513	29.225	12.740	32.376	0.50	24.40
		ATOM	1649	NE2	AHIS	513	28.916	17.908	31.176	0.50	28.30
		ATOM	1650	NE2	BHIS	513	30.334	13.396	32.081	0.50	25.54
	45	ATOM	1651	C	AHIS	513	28.666	13.164	27.738	0.50	19.81
	43			C	BHIS	513	28.720	13.171	27.738	0.50	19.42
		ATOM	1652			513					
		ATOM	1653	0	AHIS		29.601	12.426	28.026	0.50	22.45
		ATOM	1654	0	BHIS	513	29.707	12.457	27.809	0.50	22.62
	50	ATOM	1655	N	ILE	514	27.633	12.753	27.015	1.00	20.76
	30	MOTA	1656	CA	ILE	514	27.572	11.396	26.492	1.00	20.94
		ATOM	1657	CB	ILE	514	26.154	11.086	25.953	1.00	27.76
		MOTA	1658	CG2	ILE	514	26.169	9.800	25.123	1.00	28.26
		MOTA	1659	CG1	ILE	514	25.185	10.965	27.139	1.00	27.91
		MOTA	1660	CD1	ILE	514	23.752	10.649	26.753	1.00	34.31
	55	MOTA	1661	C	ILE	514	28.641	11.256	25.398	1.00	20.66
		ATOM	1662	0	ILE	514	29.298	10.226	25.285	1.00	22.21
		MOTA	1663	N	ARG	515	28.825	12.294	24.589	1.00	20.48
		ATOM	1664	CA	ARG	515	29.861	12.243	23.554	1.00	21.98
		ATOM	1665	CB	ARG	515	29.861	13.535	22.726	1.00	23.11
	60	ATOM	1666	CG	ARG	515	31.003	13.611	21.737	1.00	25.76
		ATOM	1667	CD	ARG	515	30.664	12.818	20.491	1.00	28.55
		ATOM	1668	NE	ARG	515	29.580	13.482	19.788	1.00	36.24

		5	ATOM	1669	CZ	ARG	515	29.615	13.827	18.508	1.00	38.91
			ATOM	1670	NH1	ARG	515	30.689	13.566	17.776	1.00	35.37
			ATOM	1671	NH2	ARG	515	28.579	14.459	17.971	1.00	40.27
			MOTA	1672	C	ARG	515	31.221	12.087	24.225	1.00	21.29
			ATOM	1673	ō	ARG	515	32.068	11.305	23.795	1.00	20.06
		10	ATOM	1674	N	HIS	516	31.420	12.844	25.293	1.00	23.23
		10	ATOM	1675	CA	HIS	516	32.675	12.812	26.034	1.00	24.75
					CB	HIS	516	32.566		27.206		24.73
			ATOM	1676					13.794		1.00	
			ATOM	1677	CG	HIS	516	33.826	13.948	27.990	1.00	31.42
		1.0	MOTA	1678	CD2	HIS	516	34.138	13.587	29.257	1.00	35.87
		15	MOTA	1679	ND1	HIS	516	34.938	14.586	27.489	1.00	33.59
			ATOM	1680	CE1	HIS	516	35.882	14.613	28.411	1.00	35.70
			ATOM	1681	NE2	HIS	516	35.422	14.013	29.495	1.00	33.35
			MOTA	1682	C	HIS	516	32.965	11.390	26.537	1.00	24.02
			ATOM	1683	0	HIS	516	34.059	10.852	26.362	1.00	23.66
		20	MOTA	1684	N	MET	517	31.969	10.786	27.168	1.00	20.91
			ATOM	1685	CA	MET	517	32.109	9.436	27.684	1.00	24.21
			ATOM	1686	CB	MET	517	30.837	9.038	28.424	1.00	23.88
			ATOM	1687	CG	MET	517	30.607	9.903	29.652	1.00	26.32
			ATOM	1688	SD	MET	517	29.435	9.222	30.790	1.00	26.67
	Jess.	25	ATOM	1689	CE	MET	517	27.914	9.390	29.807	1.00	23.26
	3		ATOM	1690	C	MET	517	32.399	8.448	26.564	1.00	23.26
	D		ATOM	1691	0	MET	517	33.213	7.547	26.728	1.00	26.08
	13		ATOM	1692	N	SER	518	31.736	8.612	25.423	1.00	21.93
	10		ATOM	1693	CA	SER	518	31.977	7.717	24.301	1.00	23.08
	:286	30	ATOM	1694	CB	SER	518	30.976	8.027	23.173	1.00	22.02
	+		ATOM	1695	OG	SER	518	31.283	7.336	21.978	1.00	24.01
	mb.		ATOM	1696	C	SER	518	33.432	7.862	23.810	1.00	25.15
	1		ATOM	1697	o	SER	518	34.111	6.866	23.532	1.00	22.94
	1)		ATOM	1698	N	ASN	519	33.923	9.097	23.713	1.00	22.42
	1	35	ATOM	1699	CA	ASN	519	35.295	9.309	23.260	1.00	21.87
1	į.j	55	ATOM	1700	CB	ASN	519	35.605	10.807	23.157	1.00	24.46
. 3	11		ATOM	1701	CG	ASN	519	34.864	11.469	22.021	1.00	29.02
	150		ATOM	1702	OD1	ASN	519	34.661	10.864	20.965	1.00	31.93
			ATOM	1703	ND2	ASN	519	34.459	12.715	22.224	1.00	28.81
	D	40	ATOM	1704	C	ASN	519	36.292	8.643	24.201	1.00	21.46
		10	ATOM	1705	0	ASN	519	37.251	8.015	23.752	1.00	23.56
			ATOM	1706	N	LYS	520	36.070	8.782	25.504	1.00	23.23
			ATOM	1707	CA	LYS	520	36.964	8.171	26.488	1.00	26.35
			ATOM	1708	CB	LYS	520	36.581	8.592	27.912	1.00	27.53
		45	ATOM	1709	CG	LYS	520	36.618	10.101	28.174	1.00	33.74
		45										
			ATOM	1710	CD	LYS	520	37.962	10.710	27.811	1.00	42.09
			MOTA	1711	CE	LYS	520	39.047	10.307	28.802	1.00	43.97
			MOTA	1712	NZ	LYS	520	39.858	11.480	29.254	1.00	48.07
			MOTA	1713	C	LYS	520	36.899	6.644	26.376	1.00	27.71
		50	MOTA	1714	0	LYS	520	37.913	5.957	26.501	1.00	27.15
			MOTA	1715	N	GLY	521	35.704	6.117	26.141	1.00	25.02
			MOTA	1716	CA	GLY	521	35.562	4.676	26.003	1.00	26.67
			MOTA	1717	C	GLY	521	36.254	4.168	24.753	1.00	27.06
			ATOM	1718	0	GLY	521	36.924	3.128	24.775	1.00	26.84
		55	ATOM	1719	N	AMET	522	36.101	4.893	23.650	0.50	25.87
			MOTA	1720	N	BMET	522	36.095	4.908	23.658	0.50	27.62
			MOTA	1721	CA	AMET	522	36.727	4.491	22.401	0.50	27.27
			MOTA	1722	CA	BMET	522	36.703	4.551	22.384	0.50	30.14
			ATOM	1723	CB	AMET	522	36.267	5.396	21.260	0.50	26.50
		60	MOTA	1724	CB	BMET	522	36.252	5.525	21.288	0.50	32.46
			ATOM	1725	CG	AMET	522	34.827	5.162	20.866	0.50	25.05
			MOTA	1726	CG	BMET	522	35.681	4.854	20.045	0.50	35.70

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	5	ATOM	1727	SD	AMET	522	34.585	3.587	20.020	0.50	27.07
		MOTA	1728	SD	BMET	522	34.197	5.672	19.408	0.50	40.01
		ATOM	1729	CE	AMET	522	33.142	4.017	19.031	0.50	31.29
		ATOM	1730	CE	BMET	522	34.733	6.085	17.745	0.50	42.12
		ATOM	1731	C	AMET	522	38.242	4.532	22.512	0.50	28.99
	10	ATOM	1732	C	BMET	522	38.224	4.567	22.483	0.50	30.76
		ATOM	1733	ō	AMET	522	38.939	3.743	21.870	0.50	31.65
		ATOM	1734	Ö	BMET	522	38.905	3.793	21.807	0.50	32.87
		ATOM	1735	N	GLU	523	38.749	5.452	23.324	1.00	30.85
		ATOM	1736	CA	GLU	523	40.190	5.576	23.513	1.00	34.09
	1.5										
	15	ATOM	1737	CB	GLU	523	40.515	6.725	24.480	1.00	35.59
		ATOM	1738	CG	GLU	523	40.658	8.079	23.784	1.00	43.35
		ATOM	1739	CD	GLU	523	40.560	9.265	24.739	1.00	46.63
		MOTA	1740	OE1	GLU	523	39.832	10.240	24.416	1.00	47.64
		MOTA	1741	OE2	GLU	523	41.212	9.225	25.805	1.00	43.09
	20	ATOM	1742	C	GLU	523	40.718	4.260	24.061	1.00	34.62
		ATOM	1743	0	GLU	523	41.733	3.747	23.596	1.00	33.87
		ATOM	1744	N	HIS	524	40.021	3.700	25.042	1.00	36.33
		ATOM	1745	CA	HIS	524	40.455	2.427	25.607	1.00	39.20
		ATOM	1746	CB	HIS	524	39.678	2.093	26.878	1.00	40.75
	25	ATOM	1747	CG	HIS	524	40.061	0.774	27.473	1.00	48.10
1187	20	ATOM	1748	CD2	HIS	524	41.192	0.376	28.104	1.00	48.56
115				ND1		524					
27.1		ATOM	1749		HIS		39.247	-0.338	27.412	1.00	48.84
10		MOTA	1750	CE1	HIS	524	39.859	-1.362	27.978	1.00	50.19
i sale		MOTA	1751	NE2	HIS	524	41.041	-0.956	28.407	1.00	51.61
1	30	MOTA	1752	C	HIS	524	40.290	1.282	24.613	1.00	38.06
) all		ATOM	1753	0	HIS	524	41.226	0.521	24.371	1.00	38.18
14		ATOM	1754	N	LEU	525	39.101	1.162	24.034	1.00	36.96
		ATOM	1755	CA	LEU	525	38.831	0.093	23.084	1.00	37.40
(1995		ATOM	1756	CB	LEU	525	37.416	0.241	22.514	1.00	35.89
7724	35	ATOM	1757	CG	LEU	525	36.268	0.107	23.527	1.00	33.17
luj.		ATOM	1758	CD1	LEU	525	34.936	0.246	22.811	1.00	31.77
141		MOTA	1759	CD2	LEU	525	36.343	-1.240	24.238	1.00	35.92
1		ATOM	1760	C	LEU	525	39.859	0.057	21.954	1.00	41.32
1		ATOM	1761	0	LEU	525	40.244	-1.015	21.487	1.00	40.76
9 172	40	ATOM	1762	N	TYR	526	40.314	1.227	21.522	1.00	43.68
		ATOM	1763	CA	TYR	526	41.300	1.297	20.449	1.00	49.00
		ATOM	1764	CB	TYR	526	41.376	2.722	19.890	1.00	51.86
		ATOM	1765	CG	TYR	526	42.305	2.878	18.704	1.00	57.70
		ATOM	1766	CD1	TYR	526	41.835	2.718	17.400	1.00	58.93
	45	ATOM	1767	CE1	TYR	526	42.681	2.875	16.305		61.21
	73									1.00	
		ATOM	1768	CD2	TYR	526	43.653	3.200	18.883	1.00	58.58
		ATOM	1769	CE2	TYR	526	44.510	3.359	17.790	1.00	61.15
		ATOM	1770	CZ	TYR	526	44.016	3.194	16.505	1.00	61.09
		ATOM	1771	OH	TYR	526	44.851	3.343	15.417	1.00	63.79
	50	MOTA	1772	C	TYR	526	42.671	0.871	20.964	1.00	50.14
		ATOM	1773	0	TYR	526	43.471	0.303	20.223	1.00	50.73
		ATOM	1774	N	SER	527	42.930	1.139	22.240	1.00	52.72
		ATOM	1775	CA	SER	527	44.205	0.790	22.857	1.00	55.88
		ATOM	1776	CB	SER	527	44.351	1.516	24.199	1.00	55.00
	55	ATOM	1777	OG	SER	527	43.752	0.788	25.257	1.00	52.46
		ATOM	1778	C	SER	527	44.365	-0.718	23.054	1.00	60.39
		ATOM	1779	0	SER	527	45.398	-1.185	23.534	1.00	60.43
		ATOM	1780	N	MET	528	43.335	-1.472	22.678	1.00	63.86
		ATOM	1781	CA	MET	528	43.347	-2.929	22.788	1.00	67.95
	60	ATOM	1782	CB	MET	528	42.534	-3.381	24.008	1.00	67.85
	50	ATOM	1783	CG	MET	528	41.237	-2.606	24.008	1.00	70.10
		ATOM		SD	MET	528	39.895	-3.569	24.222		71.70
		AION	1784	ענט	LIE I	220		-3.569	24.703	1.00	11.70
							253				

	5	ATOM	1785	CE	MET	528	39.231	-4.412	23.554	1.00	72.57
		ATOM	1786	C	MET	528	42.726	-3.502	21.513	1.00	70.33
		ATOM	1787	0	MET	528	42.170	-4.602	21.513	1.00	72.43
		ATOM	1788	N	LYS	529	42.834	-2.739	20.428	1.00	71.53
		ATOM	1789	CA	LYS	529	42.274	-3.122	19.136	1.00	72.00
	10	ATOM	1790	CB	LYS	529	42.508	-2.004	18.119	1.00	71.30
		ATOM	1791	C	LYS	529	42.813	-4.439	18.587	1.00	72.47
		ATOM	1792	0	LYS	529	43.990	-4.762	18.751	1.00	70.37
		ATOM	1793	N	CYS	530	41.932	-5.191	17.930	1.00	74.48
					CYS	530	42.279	-6.474	17.335	1.00	76.67
	15	ATOM	1794	CA							
	13	ATOM	1795	CB	CYS	530	41.004	-7.245	16.952	1.00	77.23
		ATOM	1796	sg	CYS	530	40.447	-8.491	18.146	1.00	79.38
		ATOM	1797	C	CYS	530	43.098	-6.220	16.065	1.00	78.08
		ATOM	1798	0	CYS	530	43.241	-5.076	15.623	1.00	78.81
		ATOM	1799	N	LYS	531	43.637	-7.289	15.487	1.00	78.22
	20	ATOM	1800	CA	LYS	531	44.424	-7.187	14.267	1.00	78.15
		ATOM	1801	CB	LYS	531	45.600	-8.182	14.305	1.00	78.33
		ATOM	1802	C	LYS	531	43.508	-7.467	13.067	1.00	77.93
		ATOM	1803	0	LYS	531	42.549	-6.734	12.839	1.00	78.07
		ATOM	1804	N	ASN	532	43.784	-8.539	12.328	1.00	77.80
(2)	25	ATOM	1805	CA	ASN	532	42.984	-8.902	11.152	1.00	77.30
AND AND		ATOM	1806	CB	ASN	532	43.550	-10.166	10.521	1.00	77.55
111		ATOM	1807	C	ASN	532	41.485	-9.082	11.423	1.00	77.34
(3)		ATOM	1808	0	ASN	532	40.904	-10.123	11.118	1.00	78.13
1.4		ATOM	1809	N	VAL	533	40.859	-8.055	11.988	1.00	76.13
4	30	ATOM	1810	CA	VAL	533	39.436	-8.098	12.280	1.00	73.77
) LL		ATOM	1811	CB	VAL	533	39.155	-7.715	13.752	1.00	73.62
1		ATOM	1812	CG1	VAL	533	39.690	-6.327	14.047	1.00	73.13
		ATOM	1813	CG2	VAL	533	37.662	-7.782	14.021	1.00	73.14
2000		ATOM	1814	C	VAL	533	38.685	-7.143	11.352	1.00	72.97
150	35	ATOM	1815	0	VAL	533	39.024	-5.960	11.252	1.00	73.91
Į,j		ATOM	1816	N	VAL	534	37.671	-7.666	10.666	1.00	70.02
U		ATOM	1817	CA	VAL	534	36.866	-6.867	9.747	1.00	66.70
E Dar		ATOM	1818	CB	VAL	534	35.619	-7.646	9.328	1.00	67.32
×Ω		ATOM	1819	C	VAL	534	36.463	-5.541	10.393	1.00	63.87
1	40	ATOM	1820	0	VAL	534	35.895	-5.519	11.486	1.00	63.55
		ATOM	1821	N	PRO	535	36.756	-4.415	9.719	1.00	60.92
		ATOM	1822	CD	PRO	535	37.424	-4.354	8.408	1.00	61.01
		ATOM	1823	CA	PRO	535	36.424	-3.077	10.229	1.00	56.83
		ATOM	1824	CB	PRO	535	36.867	-2.135	9.107	1.00	58.70
	45	ATOM	1825	CG	PRO	535	37.023	-3.009	7.893	1.00	61.55
		ATOM	1826	C	PRO	535	34.944	-2.902	10.571	1.00	52.90
		ATOM	1827	ō	PRO	535	34.067	-3.461	9.908	1.00	52.01
		ATOM	1828	N	LEU	536	34.672	-2.120	11.610	1.00	48.60
		ATOM	1829	CA	LEU	536	33.301	-1.874	12.042	1.00	45.08
	50	ATOM	1830	CB	LEU	536	33.280	-0.796	13.128	1.00	44.35
	50	ATOM	1831	CG	LEU	536	32.267	-0.750	14.273	1.00	43.48
		ATOM	1832	CD1	LEU	536	31.919	0.490	14.745	1.00	43.41
		ATOM	1833	CD2	LEU	536	31.022	-1.654	13.835	1.00	39.55
								-1.433	10.871	1.00	43.58
		ATOM	1834	C	LEU	536	32.434				
	55	ATOM	1835	0	LEU	536	31.287	-1.862	10.734	1.00	42.14
		ATOM	1836	N	TYR	537	32.992	-0.575	10.024	1.00	43.02
		ATOM	1837	CA.	TYR	537	32.269	-0.066	8.866	1.00	43.34
		ATOM	1838	CB	TYR	537	33.200	0.786	7.997	1.00	44.76
		ATOM	1839	CG	TYR	537	32.483	1.558	6.913	1.00	48.28
	60	ATOM	1840	CD1	TYR	537	32.190	0.964	5.687	1.00	48.46
		ATOM	1841	CE1	TYR	537	31.504	1.660	4.693	1.00	52.48
		MOTA	1842	CD2	TYR	537	32.073	2.875	7.123	1.00	49.99

	5	ATOM	1843	CE2	TYR	537	31.383	3.584	6.135	1.00	53.73
		MOTA	1844	CZ	TYR	537	31.100	2.967	4.924	1.00	54.01
		MOTA	1845	OH	TYR	537	30.401	3.648	3.952	1.00	55.90
		ATOM	1846	C	TYR	537	31.683	-1.199	8.032	1.00	43.15
		MOTA	1847	0	TYR	537	30.500	-1.191	7.696	1.00	41.54
	10	ATOM	1848	N	ASP	538	32.521	-2.175	7.702	1.00	44.67
	10	ATOM	1849	CA	ASP	538	32.097	-3.309	6.893	1.00	45.49
		ATOM	1850	CB	ASP	538	33.322	-4.126	6.479	1.00	51.32
		MOTA	1851	CG	ASP	538	34.361	-3.284	5.748	1.00	56.17
		MOTA	1852	OD1	ASP	538	35.436	-3.820	5.396	1.00	57.29
	15	MOTA	1853	OD2	ASP	538	34.097	-2.079	5.526	1.00	59.24
		MOTA	1854	C	ASP	538	31.071	-4.195	7.587	1.00	43.48
		ATOM	1855	0	ASP	538	30.177	-4.738	6.940	1.00	43.95
		ATOM	1856	N	LEU	539	31.193	-4.345	8.901	1.00	41.57
		ATOM	1857	CA	LEU	539	30.244	-5.157	9.654	1.00	39.11
	20	ATOM	1858	CB	LEU	539	30.734	-5.351	11.092	1.00	41.88
	20	ATOM	1859	CG	LEU	539	29.770	-6.065	12.044	1.00	46.11
				CD1	LEU	539	29.298	-7.379	11.423	1.00	46.99
		MOTA	1860								
		ATOM	1861	CD2	LEU	539	30.474	-6.319	13.377	1.00	45.76
		ATOM	1862	C	LEU	539	28.891	-4.451	9.651	1.00	36.38
10	25	MOTA	1863	0	LEU	539	27.849	-5.070	9.436	1.00	35.74
183		MOTA	1864	N	LEU	540	28.919	-3.146	9.894	1.00	35.50
113		MOTA	1865	CA	LEU	540	27.703	-2.336	9.903	1.00	35.59
1500		ATOM	1866	CB	LEU	540	28.061	-0.877	10.219	1.00	37.63
(Q -4		ATOM	1867	CG	LEU	540	27.856	-0.252	11.605	1.00	40.28
35,	30	ATOM	1868	CD1	LEU	540	27.526	-1.299	12.645	1.00	38.55
		ATOM	1869	CD2	LEU	540	29.114	0.506	11.985	1.00	41.04
frid.		ATOM	1870	C	LEU	540	27.060	-2.415	8.510	1.00	35.50
12.5		ATOM	1871	o	LEU	540	25.846	-2.585	8.371	1.00	33.21
31		ATOM	1872	N	LEU	541	27.892	-2.289	7.483	1.00	37.01
106	35	ATOM	1873	CA	LEU	541	27.418	-2.340	6.101	1.00	38.51
Lil	55					541	28.591	-2.152	5.145	1.00	39.67
1,1		ATOM	1874	CB	LEU	541	28.301	-2.112	3.643	1.00	40.92
F 154		ATOM	1875	CG	LEU						40.92
111		MOTA	1876	CD1	LEU	541	27.184	-1.130	3.348	1.00	
10		ATOM	1877	CD2	LEU	541	29.572	-1.716	2.908	1.00	44.18
1564	40	ATOM	1878	C	LEU	541	26.723	-3.676	5.833	1.00	39.75
		MOTA	1879	0	LEU	541	25.616	-3.713	5.297	1.00	36.48
		MOTA	1880	N	GLU	542	27.366	-4.770	6.230	1.00	40.88
		ATOM	1881	CA	GLU	542	26.790	-6.097	6.037	1.00	41.89
		ATOM	1882	CB	GLU	542	27.719	-7.170	6.620	1.00	44.11
	45	ATOM	1883	CG	GLU	542	27.010	-8.457	7.052	1.00	50.60
		ATOM	1884	CD	GLU	542	26.434	-9.245	5.887	1.00	55.80
		ATOM	1885	OE1	GLU	542	25.570	-10.117	6.130	1.00	58.81
		ATOM	1886	OE2	GLU	542	26.842	-8.996	4.728	1.00	57.19
		ATOM	1887	C	GLU	542	25.414	-6.195	6.691	1.00	41.58
	50			0	GLU	542	24.472	-6.720	6.102	1.00	42.82
	50	ATOM	1888						7.915	1.00	40.09
		ATOM	1889	N	MET	543	25.298	-5.686			
		MOTA	1890	CA	MET	543	24.036	-5.731	8.634	1.00	36.43
		MOTA	1891	CB	MET	543	24.270	-5.424	10.111	1.00	39.95
		MOTA	1892	CG	MET	543	25.137	-6.459	10.808	1.00	41.95
	55	ATOM	1893	SD	MET	543	24.918	-6.445	12.604	1.00	47.17
		ATOM	1894	CE	MET	543	25.324	-4.749	12.964	1.00	40.88
		ATOM	1895	C	MET	543	23.001	-4.769	8.072	1.00	35.02
		ATOM	1896	0	MET	543	21.808	-5.073	8.048	1.00	35.31
		ATOM	1897	N	LEU	544	23.457	-3.605	7.629	1.00	32.90
	60	ATOM	1898	CA	LEU	544	22.559	-2.603	7.074	1.00	36.88
		ATOM	1899	CB	LEU	544	23.225	-1.226	7.111	1.00	34.51
		ATOM	1900	CG	LEU	544	23.268	-0.562	8.490	1.00	31.94
		111 01-1	1000				_5.250		0		

	5	ATOM	1901	CD1	LEU	544	24.284	0.564	8.478	1.00	32.27
		ATOM	1902	CD2	LEU	544	21.897	-0.029	8.846	1.00	29.02
		ATOM	1903	C	LEU	544	22.148	-2.941	5.640	1.00	38.94
		ATOM	1904	o	LEU	544	20.971	-2.842	5.294	1.00	39.52
		ATOM	1905	N	ASP	545	23.118	-3.338	4.817	1.00	41.05
	10	MOTA	1906	CA	ASP	545	22.850	-3.685	3.418	1.00	40.78
		MOTA	1907	CB	ASP	545	24.159	-3.780	2.620	1.00	37.75
		ATOM	1908	CG	ASP	545	23.922	-3.937	1.120	1.00	35.19
		ATOM	1909	OD1	ASP	545	24.881	-4.265	0.380	1.00	33.48
		ATOM	1910	OD2	ASP	545	22.768	-3.734	0.691	1.00	31.33
	15	ATOM	1911	C	ASP	545	22.116	-5.015	3.349	1.00	42.87
	13			0				-6.030	2.929	1.00	44.32
		ATOM	1912		ASP	545	22.681				
		ATOM	1913	N	ALA	546	20.853	-5.009	3.755	1.00	43.49
		MOTA	1914	CA	ALA	546	20.069	-6.229	3.746	1.00	46.96
		MOTA	1915	CB	ALA	546	19.213	-6.305	5.006	1.00	47.82
	20	ATOM	1916	C	ALA	546	19.193	-6.362	2.508	1.00	49.55
		ATOM	1917	0	ALA	546	18.804	-5.368	1.883	1.00	48.75
		MOTA	1918	N	HIS	547	18.895	-7.606	2.152	1.00	50.98
		ATOM	1919	CA	HIS	547	18.042	-7.884	1.006	1.00	53.77
									0.369		52.69
	0.5	MOTA	1920	CB	HIS	547	18.431	-9.223		1.00	
(3)	25	ATOM	1921	CG	HIS	547	18.395	-10.382	1.317	1.00	55.05
		MOTA	1922	CD2	HIS	547	17.477	-10.752	2.242	1.00	53.94
		MOTA	1923	ND1	HIS	547	19.395	-11.329	1.371	1.00	56.23
177		ATOM	1924	CE1	HIS	547	19.095	-12.232	2.286	1.00	55.36
		ATOM	1925	NE2	HIS	547	17.936	-11.906	2.830	1.00	57.01
16	30	MOTA	1926	C	HIS	547	16.603	-7.936	1.518	1.00	55.69
M	00	ATOM	1927	o	HIS	547	16.362	-7.796	2.720	1.00	54.30
ļuš.				N	ARG	548	15.653	-8.139	0.612	1.00	57.00
1.4		MOTA	1928								
11		MOTA	1929	CA	ARG	548	14.245	-8.212	0.987	1.00	60.65
100		MOTA	1930	CB	ARG	548	13.432	-7.171	0.208	1.00	62.69
L.J	35	MOTA	1931	CG	ARG	548	14.272	-6.222	-0.637	1.00	67.54
Li		MOTA	1932	CD	ARG	548	13.448	-5.061	-1.171	1.00	71.92
2196		ATOM	1933	NE	ARG	548	13.702	-3.826	-0.432	1.00	76.95
1120		ATOM	1934	CZ	ARG	548	14.864	-3.178	-0.429	1.00	79.04
10		ATOM	1935	NH1	ARG	548	15.891	-3.644	-1.128	1.00	80.66
1 12	40	ATOM	1936	NH2	ARG	548	15.001	-2.063	0.278	1.00	80.39
	40	ATOM	1937	C	ARG	548	13.695	-9.608	0.711	1.00	61.65
								-9.781	0.466	1.00	62.05
		ATOM	1938	0	ARG	548	12.500				
		ATOM	1939	N	LEU	549	14.576	-10.603	0.756	1.00	62.39
		ATOM	1940	CA	LEU	549		-11.985	0.507	1.00	64.02
	45	MOTA	1941	CB	LEU	549	15.433	-12.828	0.195	1.00	62.14
		ATOM	1942	CG	LEU	549	16.461	-12.191	-0.753	1.00	60.76
		ATOM	1943	CD1	LEU	549	17.699	-13.074	-0.878	1.00	57.77
		ATOM	1944	CD2	LEU	549	15.823	-11.972	-2.108	1.00	58.38
		ATOM	1945	C	LEU	549	13.431	-12.574	1.702	1.00	66.65
	50	ATOM	1946	0	LEU	549	12.759	-13.600	1.577	1.00	67.15
	50										
		ATOM	1947	N	HIS	550		-11.920	2.856	1.00	67.72
		ATOM	1948	CA	HIS	550	12.858	-12.378	4.065	1.00	69.93
		ATOM	1949	CB	HIS	550		-12.190	5.298	1.00	70.76
		ATOM	1950	CG	HIS	550	14.977	-13.054	5.306	1.00	71.50
	55	ATOM	1951	CD2	HIS	550	15.539	-13.821	4.341	1.00	71.63
		ATOM	1952	ND1	HIS	550	15.793	-13.172	6.411	1.00	71.98
		ATOM	1953	CE1	HIS	550	16.805	-13.972	6.126	1.00	72.04
		ATOM	1954	NE2	HIS	550	16.674	-14.379	4.876	1.00	71.39
											71.15
	60	ATOM	1955	C	HIS	550	11.556	-11.603	4.275	1.00	
	60	ATOM	1956	0	HIS	550	10.940	-11.684	5.340	1.00	70.66
		ATOM	1957	N	ALA	551	11.143	-10.851	3.258	1.00	72.22
		ATOM	1958	CA	ALA	551	9.919	-10.057	3.338	1.00	73.58

	5	ATOM	1959	CB	ALA	551	9.904	-9.014	2.221	1.00	73.21
		ATOM	1960	C	ALA	551	8.658	-10.920	3.266	1.00	74.69
		ATOM	1961	0	ALA	551	7.684	-10.474	2.621	1.00	76.12
		ATOM	1962	OXT	ALA	551	8.651	-12.025	3.852	1.00	73.79
		HETATM	1963	C10	OHT	600	30.581	1.481	29.471	1.00	26.84
	10	HETATM	1964	C9	OHT	600	30.713	-0.043	29.358	1.00	22.85
	10		1965	C8	OHT	600	31.366	-0.385	28.037	1.00	25.56
		HETATM									
		HETATM	1966	C11	OHT	600	32.761	0.051	27.916	1.00	27.51
		HETATM	1967	C16	OHT	600	33.218	0.797	26.797	1.00	28.35
		HETATM	1968	C15	OHT	600	34.551	1.237	26.747	1.00	30.39
	15	HETATM	1969	C14	OHT	600	35.443	0.923	27.792	1.00	30.23
		HETATM	1970	C13	OHT	600	35.004	0.185	28.890	1.00	31.45
		HETATM	1971	C12	OHT	600	33.666	-0.241	28.955	1.00	27.93
		HETATM	1972	C7	OHT	600	30.682	-1.089	27.077	1.00	24.41
		HETATM	1973	C1	OHT	600	29.211	-1.258	27.052	1.00	24.26
	20	HETATM	1974	C2	OHT	600	28.644	-2.526	26.706	1.00	25.92
		HETATM	1975	C3	OHT	600	27.254	-2.668	26.580	1.00	26.32
		HETATM	1976	C4	OHT	600	26.438	-1.553	26.813	1.00	29.02
		HETATM	1977	04	OHT	600	25.072	-1.605	26.716	1.00	28.42
				C5		600	26.980	-0.286	27.130	1.00	26.98
	25	HETATM	1978		OHT				27.130		25.23
123	25	HETATM	1979	C6	OHT	600	28.362	-0.147		1.00	
-53		HETATM	1980	C17	OHT	600	31.370	-1.692	25.942	1.00	26.61
113		HETATM	1981	C18	OHT	600	32.508	-2.498	26.151	1.00	26.77
to		HETATM	1982	C19	OHT	600	33.166	-3.052	25.072	1.00	27.50
1,12		HETATM	1983	C20	OHT	600	32.676	-2.794	23.786	1.00	27.50
5	30	HETATM	1984	020	OHT	600	33.206	-3.566	22.795	1.00	31.35
		HETATM	1985	C23	OHT	600	33.009	-3.135	21.448	1.00	40.09
gud:		HETATM	1986	C24	OHT	600	34.226	-3.490	20.575	1.00	44.80
1		HETATM	1987	N24	OHT	600	34.141	-4.901	20.203	1.00	49.00
#1		HETATM	1988	C25	OHT	600	33.375	-5.040	18.933	1.00	51.64
1100	35	HETATM	1989	C26	OHT	600	35.495	-5.459	20.004	1.00	52.06
145		HETATM	1990	C21	OHT	600	31.540	-2.005	23.558	1.00	27.19
14.1		HETATM	1991	C22	OHT	600	30.892	-1.450	24.645	1.00	27.92
150		HETATM	1992	01	HOH	1	20.714	-12.010	23.057	1.00	27.20
40		HETATM	1993	01	нон	2	22.563	-0.070	25.819	1.00	25.77
֯	40	HETATM	1994	01	нон	3	25.183	19.202	23.149	1.00	42.52
100	40				HOH	4	35.158	5.823	37.390	1.00	33.92
		HETATM	1995	01		5		-9.922	18.914	1.00	30.18
		HETATM	1996	01	HOH		22.116				
		HETATM	1997	01	HOH	6	29.812	6.536	19.652	1.00	26.11
		HETATM	1998	01	HOH	7	13.362	4.463	20.376	1.00	29.40
	45	HETATM	1999	01	HOH	8	19.799	-11.295	20.187	1.00	28.70
		HETATM	2000	01	HOH	9	21.205	1.466	23.794	1.00	22.47
		HETATM	2001	01	HOH	10	21.177	-4.961	29.066	1.00	33.00
		HETATM	2002	01	HOH	11	18.591	1.863	20.518	1.00	32.59
		HETATM	2003	01	HOH	12	16.298	21.566	15.992	1.00	33.42
	50	HETATM	2004	01	HOH	13	18.611	1.976	24.494	1.00	29.70
		HETATM	2005	01	HOH	14	38.009	8.910	21.156	1.00	39.92
		HETATM	2006	01	HOH	15	26.549	11.664	18.080	1.00	30.25
		HETATM	2007	01	нон	16	20.282	-4.239	26.512	1.00	32.70
		HETATM	2008	01	нон	17	32.858	8.754	20.237	1.00	29.88
	55			01		18	8.497	16.136	29.934	1.00	46.80
	22	HETATM	2009		HOH				31.632	1.00	35.72
		HETATM	2010	01	HOH	19	21.940	19.301			
		HETATM	2011	01	HOH	20	35.153	2.682	14.122	1.00	41.02
		HETATM	2012	01	HOH	21	20.358	-2.268	21.013	1.00	29.43
		HETATM	2013	01	HOH	22	35.562	10.036	36.334	1.00	41.37
	60	HETATM	2014	01	HOH	23	17.248	18.187	17.571	1.00	33.96
		HETATM	2015	01	HOH	24	18.445	20.973	12.346	1.00	43.44
		HETATM	2016	01	HOH	25	12.152	23.054	33.132	1.00	36.04

	5	HETATM	2017	01	HOH	26	1	13.181	22.222	9.699	1.00	37.03
		HETATM	2018	01	HOH	27	1	19.399	-6.090	12.808	1.00	44.86
		HETATM	2019	01	HOH	28	3	37.895	13.599	31.395	1.00	47.26
		HETATM	2020	01	HOH	29	1	1.570	6.212	7.962	1.00	51.10
		HETATM	2021	01	HOH	30	2	20.172	-2.568	23.445	1.00	51.70
	10	HETATM	2022	01	HOH	31	3	36.402	-5.369	23.729	1.00	58.20
		HETATM	2023	01	HOH	32	2	25.127	13.802	19.187	1.00	35.29
		HETATM	2024	01	HOH	33	2	23.181	4.937	38.538	1.00	33.77
		HETATM	2025	01	HOH	34	2	20.550	0.421	21.276	1.00	29.12
		HETATM	2026	01	HOH	35	3	39.599	13.954	27.312	1.00	44.08
	15	HETATM	2027	01	HOH	36	- 2	26.445	13.863	21.285	1.00	34.97
		HETATM	2028	01	HOH	37	1	L3.759	5.079	9.108	1.00	38.54
		HETATM	2029	01	HOH	38	- 1	L4.150	24.731	34.529	1.00	49.72
		HETATM	2030	01	HOH	39	2	21.060	13.886	-6.319	1.00	59.79
		HETATM	2031	01	HOH	40	3	32.215	6.217	8.726	1.00	60.22
	20	HETATM	2032	01	HOH	41	3	35.105	15.704	9.069	1.00	45.15
		HETATM	2033	01	HOH	42	1	1.427	19.451	9.903	1.00	38.56
		HETATM	2034	01	нон	43	1	19.662	23.472	10.333	1.00	47.71
		HETATM	2035	01	нон	44		9.231	3.690	12.337	1.00	45.98
		HETATM	2036	01	HOH	45	1	15.313	-6.036	17.192	1.00	39.07
1755	25	HETATM	2037	01	нон	46	3	15.517	-3.266	17.907	1.00	37.67
250		HETATM	2038	01	HOH	47	2	28.784	-16.713	25.163	1.00	55.44
+ <u>L</u> I		HETATM	2039	01	HOH	48	2	27.868	-10.898	28.271	1.00	31.27
17.		HETATM	2040	01	HOH	49		6.955	13.568	28.233	1.00	48.83
(0		HETATM	2041	01	нон	50	2	22.051	-15.030	28.603	1.00	36.91
1 miles	30	HETATM	2042	01	HOH	51		7.026	31.002	30.284	1.00	46.73
N		HETATM	2043	01	HOH	52		1.489	12.385	15.164	1.00	51.17
[mb		HETATM	2044	01	HOH	53		3.499	6.444	14.452	1.00	50.38
4		HETATM	2045	01	HOH	54	1	L8.655	-2.048	25.518	1.00	52.29
15		HETATM	2046	01	HOH	55	2	28.188	-15.195	38.996	1.00	55.22
تما	35	HETATM	2047	01	HOH	56	2	35.275	-10.556	38.061	1.00	57.39
1.4		HETATM	2048	01	HOH	57		37.771			1.00	54.17
		HETATM	2049	01	HOH	58	3	31.403			1.00	46.80
1		HETATM	2050	01	HOH	59		30.455			1.00	47.05
100		HETATM	2051	01	HOH	60		25.985		0.416	1.00	43.32
10	40	HETATM	2052	01	HOH	61		35.679			1.00	42.99
		HETATM	2053	01	HOH	62		L4.741			1.00	49.59
		HETATM	2054	01	HOH	63		L6.333			1.00	45.13
		HETATM	2055	01	HOH	64		23.809			1.00	45.36
		HETATM	2056	01	HOH	65		27.012			1.00	63.39
	45	HETATM	2057	01	HOH	66		25.956			1.00	44.94
		HETATM	2058	01	HOH	67		23.510			1.00	39.06
		HETATM	2059	01	HOH	68		11.475			1.00	55.50
		HETATM	2060	01	HOH	69		36.519			1.00	41.56
		HETATM	2061	01	HOH	70		30.111			1.00	44.58
	50	HETATM	2062	01	HOH	71		26.850			1.00	40.15
		HETATM	2063	01	HOH	72		20.448			1.00	42.50
		HETATM	2064	01	HOH	73	3	33.896			1.00	46.39
		HETATM	2065	01	HOH	74	- 1	16.884			1.00	61.50
		HETATM	2066	01	HOH	75		18.595	0.296	27.866	1.00	47.33
	55	HETATM	2067	01	HOH	76		6.166			1.00	47.94
		HETATM	2068	01	HOH	77	- 1	L8.484			1.00	35.52
		HETATM	2069	01	HOH	78		1.985			1.00	46.42
		HETATM	2070	01	HOH	79	- 1	L2.729	30.461	27.530	1.00	62.79
		END										

METHODS AND COMPOUNDS FOR MODULATING NUCLEAR RECEPTOR COACTIVATOR BINDING

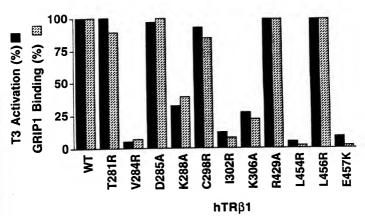
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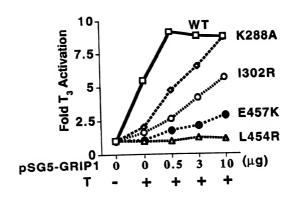
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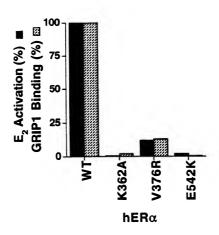
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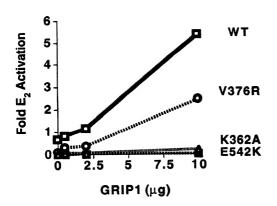
ABSTRACT OF THE DISCLOSURE

The present invention relates to methods and agonist/antagonist compounds for modulating nuclear receptor coactivator binding. The invention includes a method for identifying residues comprising a coactivator binding site for a nuclear receptor of interest. Also included is a method of identifying agonists and/or antagonists that bind to a coactivator binding site of a nuclear receptor of interest. Agonists and antagonists of coactivator binding to nuclear receptors also are provided. The invention is exemplified by identification and manipulation of the coactivator binding site of the thyroid receptor (TR), and compounds that bind to this sites. The methods can be applied to other nuclear receptors including RAR, RXR, PPAR, VDR, ER, GR, PR, MR, and AR.









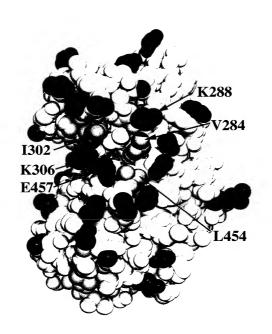


FIG. 5

Nuclear

CBP & p300

PAS Transcriptional

Receptor interaction

interaction

activation domain AEGHSRLHDSKGQTKLLQLLTTKSEQMEPSPLAS SEO ID NO: 5 Grip1 SEO ID NO: 8 Tif2 ADGOSRLHDSKGOTKLLOLLTTKSEOMEPSPLAS SEQ ID NO: 11 NcoA-2 AEGHSRLHDSKGQTKLLQLLTTKSEQMEPSPLPS SEO ID NO: 14 RAC3 AENQRGPLESKGHKKLLQLLTCSSEDRGHSSLTN SEO ID NO: 17 AIB1, TRAM-1 AENORGPLESKGHKKLLOLLTCSSDDRGHSSLTN SEQ ID NO: 20 p/CIP SETPRGPLESKGHKKLLQLLTCSSEDRGHSSLTN SEQ ID NO: 23 SRC1 SEGDSKY -- SQTSHKLVQLLTTTAEQQLRHADID SEO ID NO: 26 Consensus .-.....S....KLhOLLT...-.... SEO ID NO: 6 Grip1 PGSTHGTSLKEKHKILHRLLODSSSPVDLAKLTA SEO ID NO: 9 Tif2 SGSTHGTSLKEKHKILHRLLODSSSPVDLAKLTA SEQ ID NO: 12 NCOA-2 PGSTHGTSLKEKHKILHRLLQDSSSPVDLAKLTA SEO ID NO: 15 RAC3 TSNMHGSLLOEKHRILHKLLONGNSPAEVAKITA SEO ID NO: 18 AIB1, TRAM-1 TSNMHGSLLQEKHRILHKLLQNGNSPAEVAKITA SEQ ID NO: 21 p/CIP TSNVHGSLLOEKHRILHKLLONGNSPAEVAKITA SEO ID NO: 24 SRC1 TCPSSHSSLTERHKILHRLLOE.GSPSDITTLSV SEQ ID NO: 27 ConsensusL.E+H+ILH+LLQ...SP.-h..h.. SEO ID NO: 7 Grip1 EPASPKKKE---NALLRYLLDKDDTKDIGLPEIT SEQ ID NO: 10 Tif2 EPVSPKKKE---NALLRYLLDKDDTKDIGLPEIT SEO ID NO: 13 NcoA-2 EPASPKKKE---NALLRYLLDKDDTKDIGLPSIT SEO ID NO: 16 RAC3 EQLSPKKKE - - NNALLRYLLDRDDPSDVLAKKLQ SEQ ID NO: 19 AIB1, TRAM-1 EQLSPKKKE -- NNALLRYLLDRDDPSDALSKELQ SEO ID NO: 22 p/CIP EOLSPKKKE -- NNALLRYLLDRDDPSDALSKELO ELDAAKKKESKDHQLLRYLLDKDEKDLRSTPNLC SEO ID NO: 25 SRC1 SEQ ID NO: 28 Consensus E...KKKE....LLRYLLD+D-....h. Overall Consensus (SEO ID NO: 1)

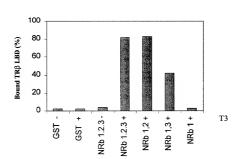
Nuclear Receptor

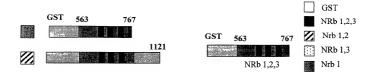
CBP & p300 interaction interaction

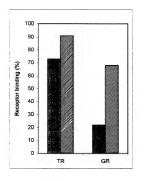
bHLH PAS Transcriptional

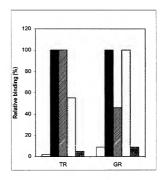
NRb 1

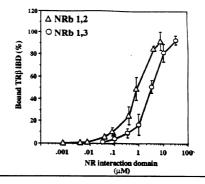
activation domain predicted a-helices GST NR-box1 NR-box1 NR box3 residues 15-21 residues 15-21 residues 15-21 SEQ ID NO: 5 SEQ ID NO: SEQ ID NO: 7 NRb 1,2,3 KLLQLLT.ILHRLLQ. . .LLRYLLD NRb 1,2 NRb 1,3 KLLOLLT. AAHRAAO. LLRYLLD

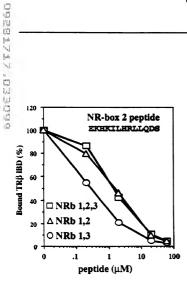


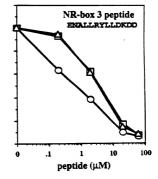


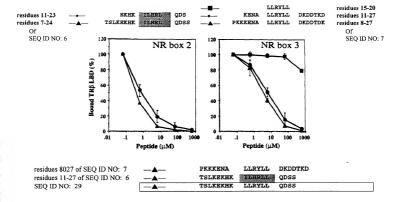


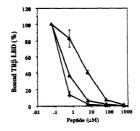


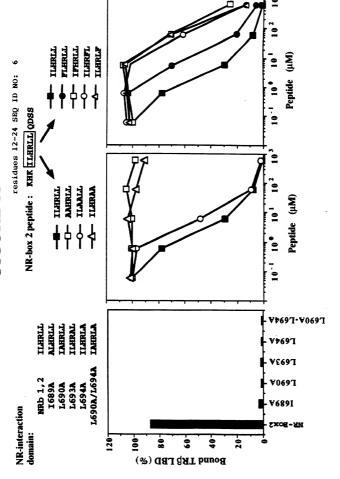












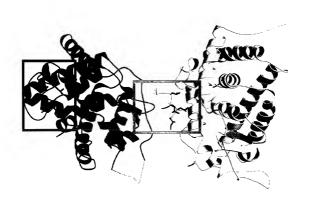


FIG. 12

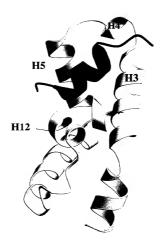


FIG. 13

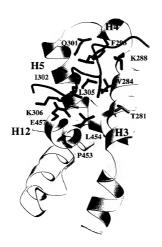


FIG. 14

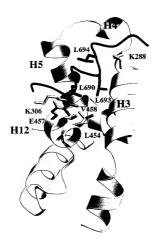


FIG. 15

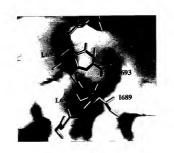


FIG. 16

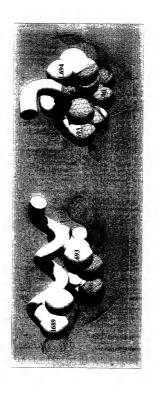


FIG. 17

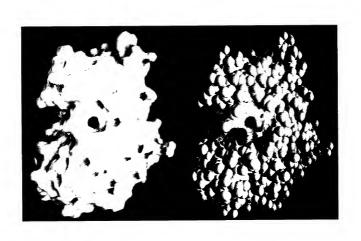


FIG. 18

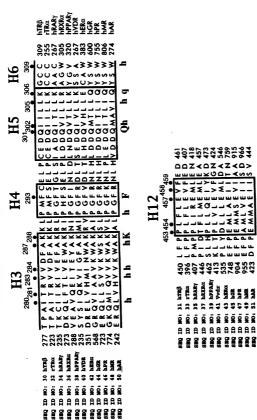


FIGURE 19